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16. KEY

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7. Abstract

This thermal analysis determines transient temperature distributions in and around a grout storage vault containing the M-106.3 formulation of grout. When poured at an initial grout temperature of 40°C, the maximum grout temperature criterion of 90°C is not exceeded. In addition, the base radiolytic heat generation rate of 260 curies/cubic meter can be increased by 35% before the maximum grout temperature reaches 90°C.

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GROUT VAULT HEAT TRANSFER RESULTS FOR M-106 GROUT FORMULATION

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October 1990

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Technology

ACKNOWLEDGEMENT

John C. Guzek provided consultation and checking during the development stages of the TAPA computer model.

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<u>Figures:</u>

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TABLES:

1.0 INTRODUCTION

Many waste stabilization criteria and standards exist for the safe disposal of radioactive wastes. The regulations require a certain performance by the waste disposal system. Part of the required performance for disposal of waste by using the grout process is its thermal behavior. If the grout gets too hot from the hydration and radiolytic heat, its performance will deteriorate and not meet waste stabilization criteria.

This report presents the results of a transient thermal analysis of a grout vault containing the M-106.3 grout formulation for use on the waste contained in the underground storage tank 106-AN. The purpose of the study is to provide temperature data throughout the vault structure using a representative grout formulation which can be used for stress analysis calculations. In addition, an analysis is investigated which shows the temperature affect of grout radionuclide content. This information can be used to maximize the radionuclide content without exceeding peak temperature constraints.

A two- and three-dimensional TAPA (Reference 1) computer model was developed to analyze the problem. The suitability of using each model is discussed.

This report is organized as follows. Section 2 describes the computer code, the models developed, and all assumptions associated with the models; Section 3 and 4 describes the results of the analysis; Section 5 summarizes the conclusions; and Appendix A describes the controlling software required to complete the problem.

2.0 CODE AND MODEL DESCRIPTION

2.1 TAPA COMPUTER CODE QUALITY ASSURANCE

The TAPA computer code was used to model the heat transfer problem. This code is a generalized finite difference code capable of modeling arbitrary geometry configurations. The code was originally developed at the Westinghouse Astronuclear Laboratory by B. L. Pierce in 1969. Since then, it has been used extensively at Hanford and has completed the software quality assurance requirements for level 2 QA applications (Reference 1). Configuration control requirements, as outlined in the QA manual WHC-CM-4-2, Section QI 3.3, Rev. 1, have been met and the study complies with the engineering practice EP-2.1, Rev. 2 computer software configuration management.

Both two- and three-dimensional models were created. The model descriptions are separated into two-dimensional (2D) and three-dimensional (3D) physical descriptions. The final section describes all additional assumptions common to both configurations.

2.2 TWO-DIMENSIONAL MODEL

Figure 1 shows the physical dimensions of the two-dimensional model. This model shows a unit thickness slice through the center of a grout vault assuming an infinite array of grout vaults whose center-to-center vault spacing is 86.5 feet. The material makeup of the regions and location of the boundary conditions are also shown in Figure 1. The total number of node points is 300. The applicability of using each model will be discussed later.

An actual grout vault contains three additional layers between the outside concrete wall and asphalt. A geogrid material is next to the concrete which allows water to drain down the outer wall. The next layer is a plastic liner for leak sealing, and a third layer is an insulating board which protects the plastic layer from the hot asphalt during construction. These layers were not modeled because of the extra model complexity of adding these very narrow regions to the existing model. By disregarding these layers, the temperature gradient across the concrete walls will be higher, thus giving conservative estimates for stress analysis calculations.

2.3 THREE-DIMENSIONAL MODEL

The three-dimensional model is shown in Figure 2. The model assumes an infinite array of grout vaults whose side-to-side center-to-center spacing is 86.5 feet and whose end-to-end center-to-center spacing is 161 feet. The x-z dimension is the same as the two-dimensional model. The y dimension is broken into seven slices. Three slices represent one half of a grout vault, a fourth slice represents the two foot thick concrete end wall of the vault, and slices 5 through 7 represents the soil at the end of the grout vault. The material makeup and location of applicable boundary conditions are also shown on Figure 2. The total number of node points is 2100.

As discussed in the two-dimensional model previously, the three-dimensional model does not include the three layers between the concrete and asphalt either.

2.4 COMMON MODEL ASSUMPTIONS

The physical properties used for this study are shown in Table 1. The TAPA input units based on inches and seconds are shown in addition to the more familiar hour and feet units for density and thermal conductivity.

Three boundary conditions were used on the edge of the model as shown in Figure 1. A 55°F isothermal boundary condition exists at the soil-water table interface represented at $z = 0$ on the model. An adiabatic boundary condition exists at $x = 43.25$ feet which approximates an infinite array of grout vaults whose side-to-side center-to-center spacing is 86.5 feet. A forced convection and radiation boundary condition exists at the soil-air interface at $z=256.41$ feet. The forced convective coefficient is 0.78 BTU/(hr-Ft^2-°F) convecting to

80°F. This was based on a heat transfer coefficient that was obtained from the Nusselt number (Nu) correlation below of Grashof number (Gr) and Prandtl number (Pr) for free convection turbulent flow:

$$Nu = C\ [(Gr)(Pr)]^{1/3}$$

The value of "C" ranges from 0.104 (Reference 2) to 0.13 (Reference 3), and in turn is multiplied by 1.65 for application to a horizontal surface (Reference 4). The radiation boundary condition assumes the soil surface to be a gray body whose emissivity is 0.8. An additional adiabatic boundary condition exists at z = 80.5 feet which approximates an infinite array of grout vaults whose end-to-end center-to-center spacing is 161 feet.

The heat transfer mechanism in the air region inside the grout vault above the grout surface was assumed to be radiation and natural convection. TAPA has no mechanism to model a true natural convection mechanism, so a thermal conductivity of ten times the stagnant air thermal conductivity was used as a conservative approximation. Effective heat transfer using a conduction factor that is obtained assuming natural convection for a unity gap dimension indicates a factor of about 20 in the vertical direction and in a large plenum could be orders of magnitude greater. In the lateral direction however, the heat transfer is notably less in which this factor ranges between only about 10 or 20 (Reference 5).

The heat released due to the heat of hydration was derived from Reference 6 which measured the adiabatic heatup of a sample of grout as it cured. Errors associated with the experiments make the experimental temperatures measured at the end of the test ±5°C (Reference 7). Adiabatic conditions are assumed over the short term time period when the heat of hydration is released which allows the data in Reference 6 to be used directly as the heat of hydration data. A two-dimensional model of a transient adiabatic heatup was used to calibrate the model so the temperatures predicted by the model were identical to the measured laboratory data. By multiplying the actual heat of hydration rates by 0.99, the adiabatic model heatup results were identical to the actual measured results. In addition to the heat of hydration, the radiolytic heat generation rate must be considered. The radiolytic heat is considered to be generated by cesium 137 at a heat loading of 260 Curies/cubic meter (Reference 8). Cesium 137 is the most dominating heat generation element and using this assumption will give conservatively high temperatures. Both heat generation rates are tabulated in Table 2.

A grout vault is filled with grout whose initial temperature is 104°F to an elevation of 30 feet in a continuous pour lasting for 400 hours. Because the computer model cannot handle a moving boundary condition, the continuous pour was broken into 20 discrete pours, each of 1.5 foot thickness, lasting for 20 hours. During the vault filling, the asphalt concrete covering the cover block is exposed to the atmosphere. Three months after the vault is filled, the air space above the grout is filled with nonradioactive grout whose heat of hydration and initial pour temperature is equal to the radioactive grout. The asphalt over the cover block is then backfilled with soil.

The temperature limit established to ensure long-term grout stability is 90°C. This limit is based on precluding the boiling of water in the grout monolith and the preparation and curing of grouts at elevated temperatures. Laboratory tests show that grouts with acceptable physical properties are obtained at temperatures up to 100°C (Reference 9). The experimentally determined temperature limit of 100°C is reduced by 10°C to give the operating temperature limit of 90°C. This temperature limit is applied during both the grout processing and setting period and the long-term disposal period after the grout has cured.

3.0 HEAT TRANSFER RESULTS

Two-dimensional model results are discussed in Section 3.1 and three-dimensional model results are discussed in Section 3.2.

3.1 TWO-DIMENSIONAL MODEL RESULTS

Results from the two-dimensional model are broken into four areas: the relative effects of the heat of hydration and radiolytic heat loads, the maximum center line temperatures, temperature drops through the vault structure, and temperature contour plots. Each of these areas are discussed below.

Maximum grout temperatures are shown in Figure 3. The three curves illustrate the relative contribution of the hydration heat and the radiolytic heat to the combined hydration plus radiolytic generation. To expand the curve during the grout pouring, a 0 to 1 year time scale is shown in Figure 4. Comparison of the hydration + radiolytic heat curve with the hydration only curve shows that the radiolytic heat generation rate has little effect on the maximum initial peak, but the second peak is controlled almost entirely by the radiolytic heat content.

The maximum grout centerline temperature at selected grout elevations is shown in Figure 5. This shows the centerline temperature as a function of time at three elevations in the vault. The ending time is at the point where the asphalt over the cover block is back filled with soil. As shown, the maximum centerline temperature of 194°F occurring 1880 hours after time zero occurs within the grout pour rather than at the bottom of the pour. The temperature peak at the top of the grout is due to the pouring of the top layer of grout at 400 hours.

Temperature drops from the inside of the vault to the soil surrounding the vault are shown in Figures 6 through 13. Each of these figures shows a temperature drop from the inner vault structure to the soil surrounding the vault at various locations on the structure. Figure 14 shows a detailed map of the point positions shown in Figures 6 through 13. Figure 6 shows the centerline temperature drop at the floor of the vault. Figure 7 shows the temperature drop on the floor of the vault through the bottom where the floor meets the wall. Figure 8 shows the temperature drop out the side of the wall where the vault wall meets the floor. Figure 9 shows the temperature drop in the wall at a grout height of 15 feet. Figure 10 shows the temperature drop in the wall at a grout height of 30 feet. Figure 11 shows the temperature drop in the wall where the wall meets the roof. Figure 12 shows the centerline temperature drop across the concrete coverblock. Figure 13 shows the temperature drop through the concrete at the edge of the coverblock. The temperature spike in Figures 12 and 13 are due to the last grout pour at 400 hours.

A variation of the wall temperatures shown in Figures 9 through 11 are shown in Figures 15 and 16. Figure 15 shows the inside and outside vault wall temperature along its height for a full vault (time = 400 hours). Figure 16 shows temperatures at the same location when the maximum temperature due to the grout heat of hydration occurs (1880 hours).

Figure 17 and 18 shows the maximum centerline to edge temperatures as a function of vault height. Figure 17 presents the data when the grout vault is full (400 hours) and Figure 18 presents the data at the same location when the maximum temperature due to the grout heat of hydration occurs.

Temperature contour plots can be used to illustrate the temperature distribution throughout the two-dimensional model. Figure 19 shows a temperature contour plot at a time period of 400 hours, the time when the vault is completely filled. As a comparison, Figure 20 shows the same plot at a time period of 2560 hours or three months after being filled. As shown, the heat has spread out both horizontally and vertically in Figure 20. The contour plots were plotted by a contour plotting package (Reference 10); further documentation on this package is contained in Appendix A.

3.2 THREE-DIMENSIONAL MODEL RESULTS

The three-dimensional model was developed to verify the results of the two-dimensional model. Figure 21 shows a linear plot of the maximum grout temperatures as a function of time for the two- and three-dimensional models. To expand the grout filling time periods, a time scale of 0 to 1 year is shown in Figure 22. As shown, the two models agree within approximately 4°F for about the first year, but for the long term heat predictions, temperatures predicted by the three-dimensional model are up to 15°F lower than the two-dimensional model. The same boundary conditions were used for both the two-and three-dimensional models so the "level of conservatism" is the same in both cases. The difference is solely due to the extra soil modeled at the end of the grout vault. This extra soil volume in the three-dimensional model gives a larger initial heat sink for heat transfer and also provides additional surface area to transfer heat at the soil-air interface. These results show that the two-dimensional model can be used to adequately model scenarios up to about a year, but for long term temperature predictions, the three-dimensional model is necessary to predict accurate temperatures.

The second temperature peak which is due to the radiolytic heat content is lower than the initial temperature peak for the base case radiolytic heat loading of 260 curies/cubic meter Because the radiolytic heat content has little effect on the initial temperature peak, additional radiolytic heat can be stored in the grout providing the second temperature peak does not exceed the first peak. Figure 23 shows a linear scaled plot presenting the results of varying the radiolytic generation rate from the base rate of 260 curies/cubic meter to 50 percent above this base rate. Figure 24 shows the same plot with a log time axis so the initial grout filling history can be also seen. As shown earlier, the radiolytic heat rate has little affect on the first peak. This graph also shows that the radiolytic heat generation rate can be increased 35 percent above the base value and still produce a second temperature peak no greater than the first peak. Increasing the radiolytic heat load could have significant cost savings by decreasing the number of vaults required.

4.0 CONCLUSIONS

The results of this heat transfer analysis show that the M-106 grout formulation, when poured at an initial temperature of 104°F, will not exceed the maximum grout temperature criterion of 90°C.

Comparison of the 2D and 3D model results show that the 2D model is suitable only for temperature predictions out to about one year; the maximum temperature difference at one year being 4°F. For long term temperature predictions, the 3D model must be used. The temperatures predicted by the 3D model are approximately 15°F lower than the 2D model in the 5 to 50 year time range.

Two maximum temperature peaks occur in this system. The first peak occurs relatively shortly after the grout vault is filled and is caused primarily by the heat of hydration in the grout formulation. The second temperature peak which occurs about 15 years after the vault has been filled is controlled by the grout radiolytic heat content. Since the first temperature peak is controlled almost solely by the heat of hydration, the radiolytic heat content can be increased until the second temperature peak approaches the initial first peak. Results of the 3D model shows that approximately 35% more radiolytic heat can be stored in the grout mixture without exceeding the initial first temperature peak.

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2. J. C. Guzek and D. L. Polzin, Evaluation of Natural Convection Air Cooling Test in FFTF Interim Decay Storage Vessel, HEDL-TC-2683 (June 1985).

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5. J. C. Petrie, et.al., Radiative and Convective Heat Transfer Within Vertical Annular Spaces Open at the Ends, INEL Report Number IN-1110 (December 1967).

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7. Meeting Minutes, Heat of Hydration of the Re-Formulated Grout, S. S. Chang/R. D. Claghorn to attendees, January 22, 1990.

8. V. W. Thomas, et.al., Interim Criteria and Standards for Disposal of Grouted Waste at Hanford, PNL 6339 UC-70, September 1987.

9. DOE/RL 88-27, Rev. 1, Grout Treatment Facility Dangerous Waste Permit Application, Part B, January 17, 1990.

10. SURFER, Version 4, Golden Software, Inc.

Table 1 Model Physical Properties

	DENSITY		THERMAL CONDUCTIVITY		HEAT CAPACITY
Material	Lbs/Ft^3	Lbs/In^3	Btu/(Hr x Ft°F)	Btu/(Sec x In°F)	BTU(lb°F)
Concrete[1]	144	0.08333	0.7	1.62×10^{-5}	0.21
Grout[2]	104.2	0.0603	0.5314	1.23×10^{-5}	0.49
Asphalt[3]	131.33	0.076	0.0994	2.3×10^{-6}	0.22
Gravel[4]	100.22	0.058	0.1382	3.2×10^{-6}	0.2
Soil[5]	126.14	0.073	0.2894	6.7×10^{-6}	0.22
Air[1]	0.0651	0.000035	0.0167	3.3×10^{-7}	0.241
Rebar[6]	490.75	0.284	27.0	6.25×10^{-4}	0.112

(1) "Fundamentals of Momentum, Heat, and Mass Transfer", Welty, Wicks, Wilson, 1969, John Wiley and Sons, Inc.
(2) Internal Memo, J. H. Westik Jr., to J. A. Voogd, HGTP-90-013, January 31, 1990 (see Appendix B).
(3) WHC-SD-WM-ER-082, "Asphalt Diffusion Break and Barrier Material Properties", W. J. Powell, August 31, 1990.
(4) Marts Standard Handbook for Mechanical Engineers, 8th Edition, McGraw Hill.
(5) J. C. Petrie, et.al., "Radiative and Convective Heat Transfer Within Vertical Annular Spaces Open at the Ends", INEL Report Number IN-1110 (December 1967).
(6) "ASHRAE Handbook of Fundamentals", American Society of Heating, Refrigerating and Air Conditioning Engineers, Inc., 1972.

Table 2 Grout Heat Generation Rate

Time (Hours)	Heat Generation Rate: Hydration* BTU/(Hr x Ft^3)	Radiolytic** BTU/(Hr x Ft^3)
20	7.444	0.121
40	9.053	
60	64.149	
80	15.21	
100	9.742	
120	8.501	
140	7.812	
160	7.398	
180	6.066	
200	5.239	
220	5.009	
240	4.963	
260	5.285	
280	5.560	
300	5.1007	
320	4.5493	
340	4.183	
360	3.630	
380	3.998	
400	3.355	
450**	2.959	
500	2.334	
550	2.187	
600	2.004	
650	1.875	
700	1.765	
750	1.654	
800	1.140	
801	0	

* Hydration heat generation rates above 450 hours calculated by a power curve fit ($y = ax^b$) of the actual data points between 400 and 470 hours and an endpoint of 194°F. Data from Reference 6.

** Assuming: 260 Ci/m^3 Cs^{137}
30.17 year half life
0.0164 BTU/(Hr x Ci)
$Q = 0.121e^{-2.62268 \times 10^{-6} \cdot t}$ when t is time in hours
Data from Reference 8.

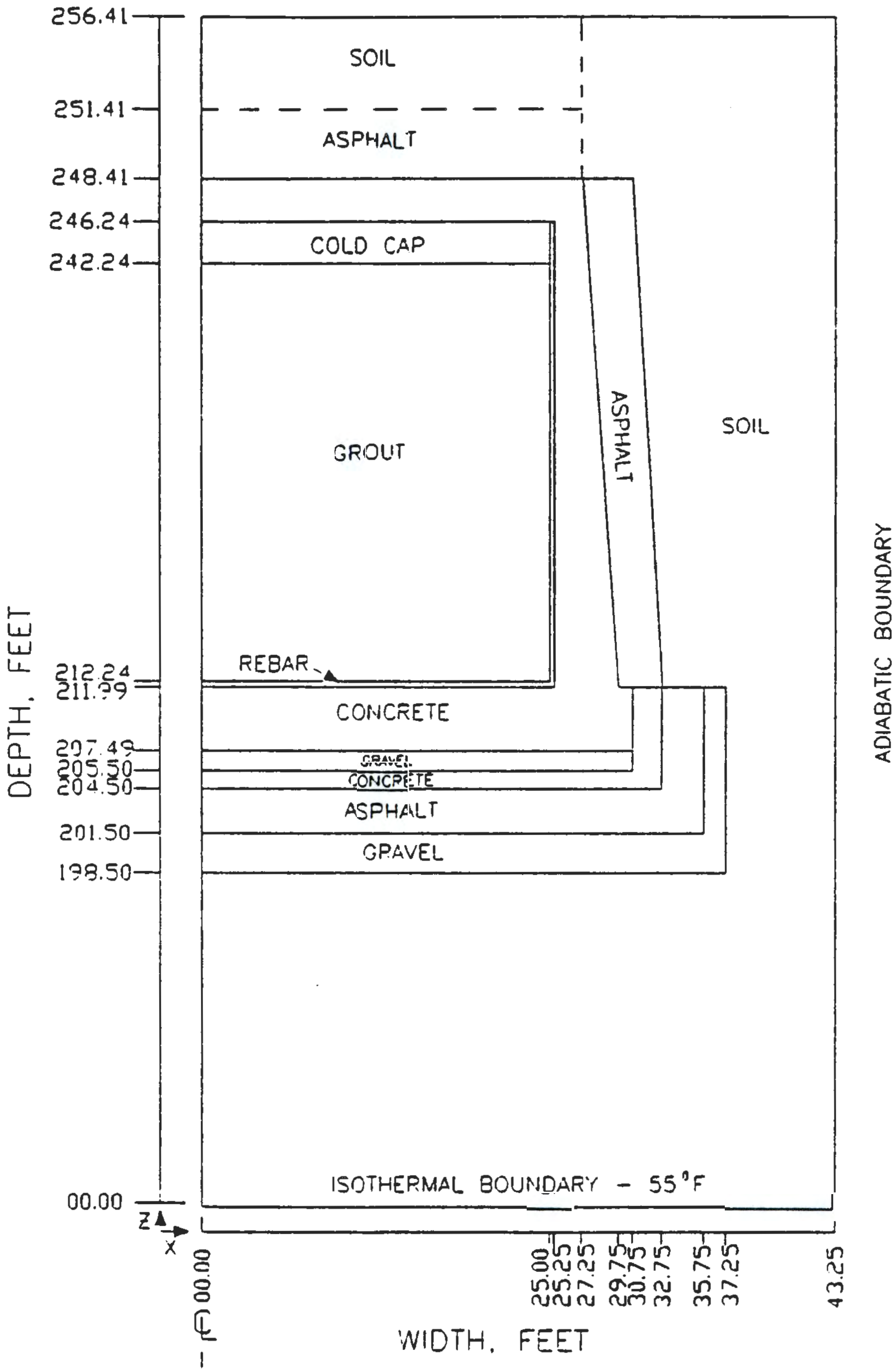

Figure 1. Asphalt Barrier Grout Vault, 2-Dimensional Model.

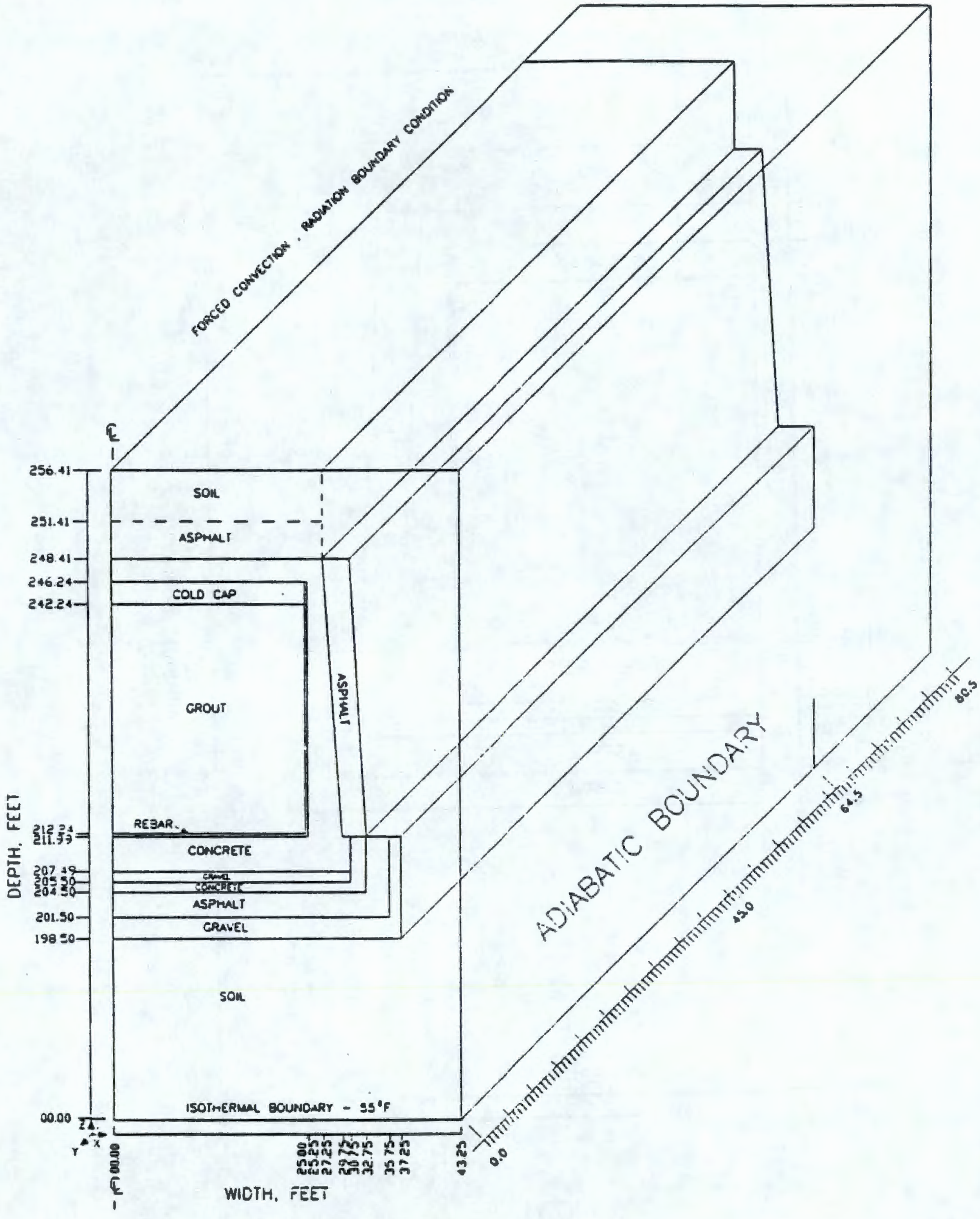

Figure 2. Asphalt Barrier Grout Vault, 3-Dimensional Model.

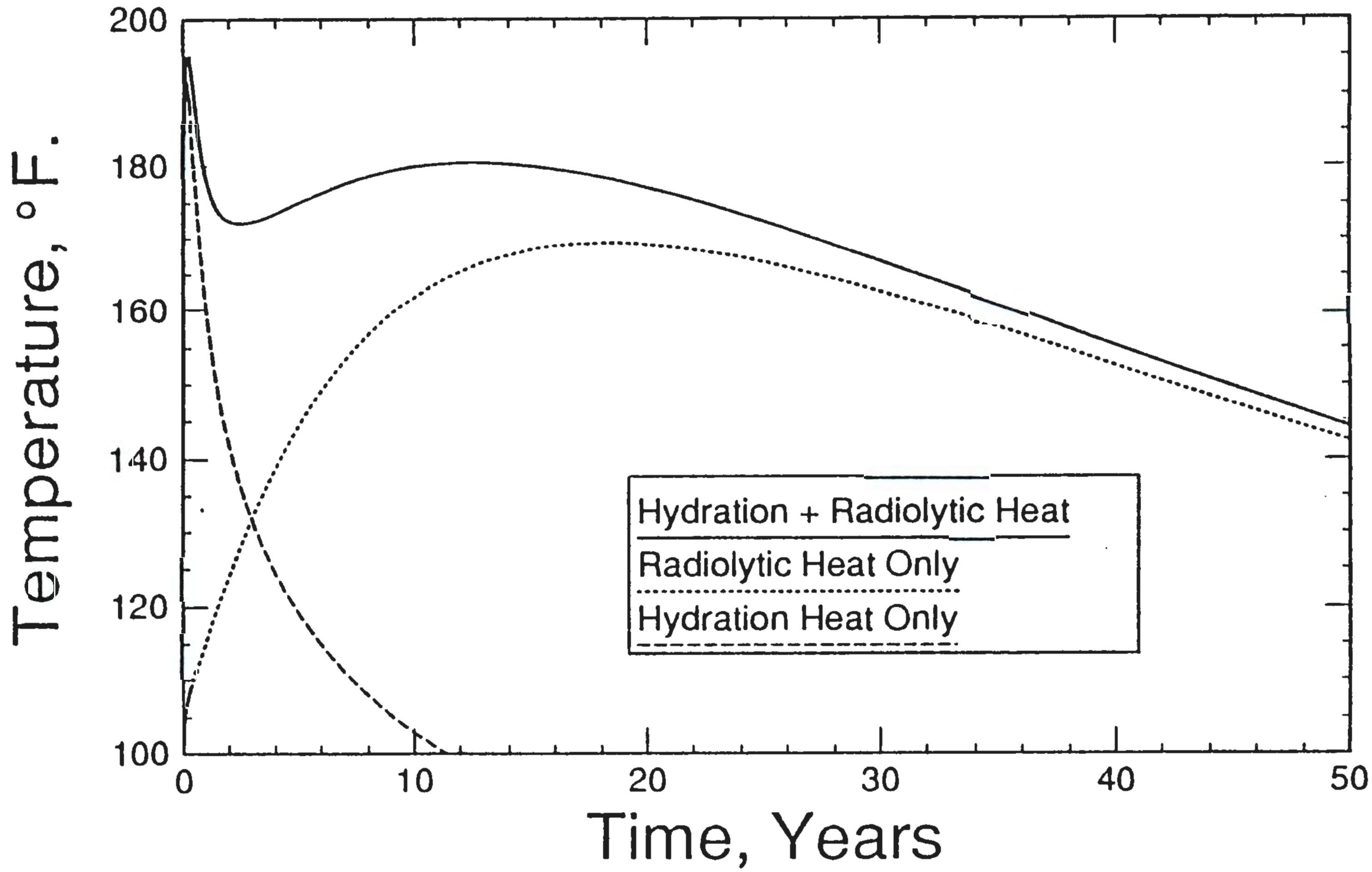

Figure 3. Maximum Grout Temperature, 2-Dimensional Model

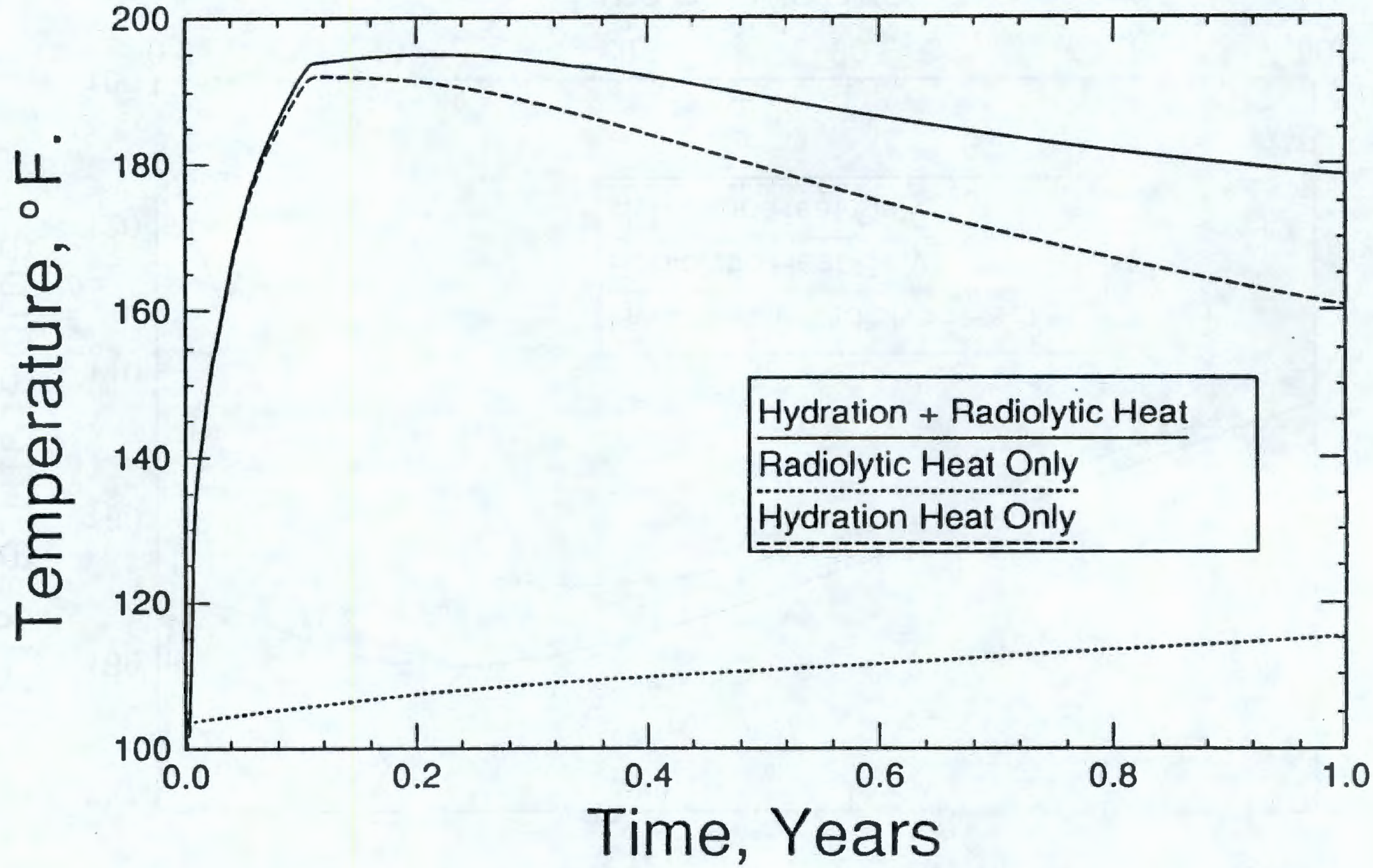

Figure 4. Maximum Grout Temperature, 2-Dimensional Model

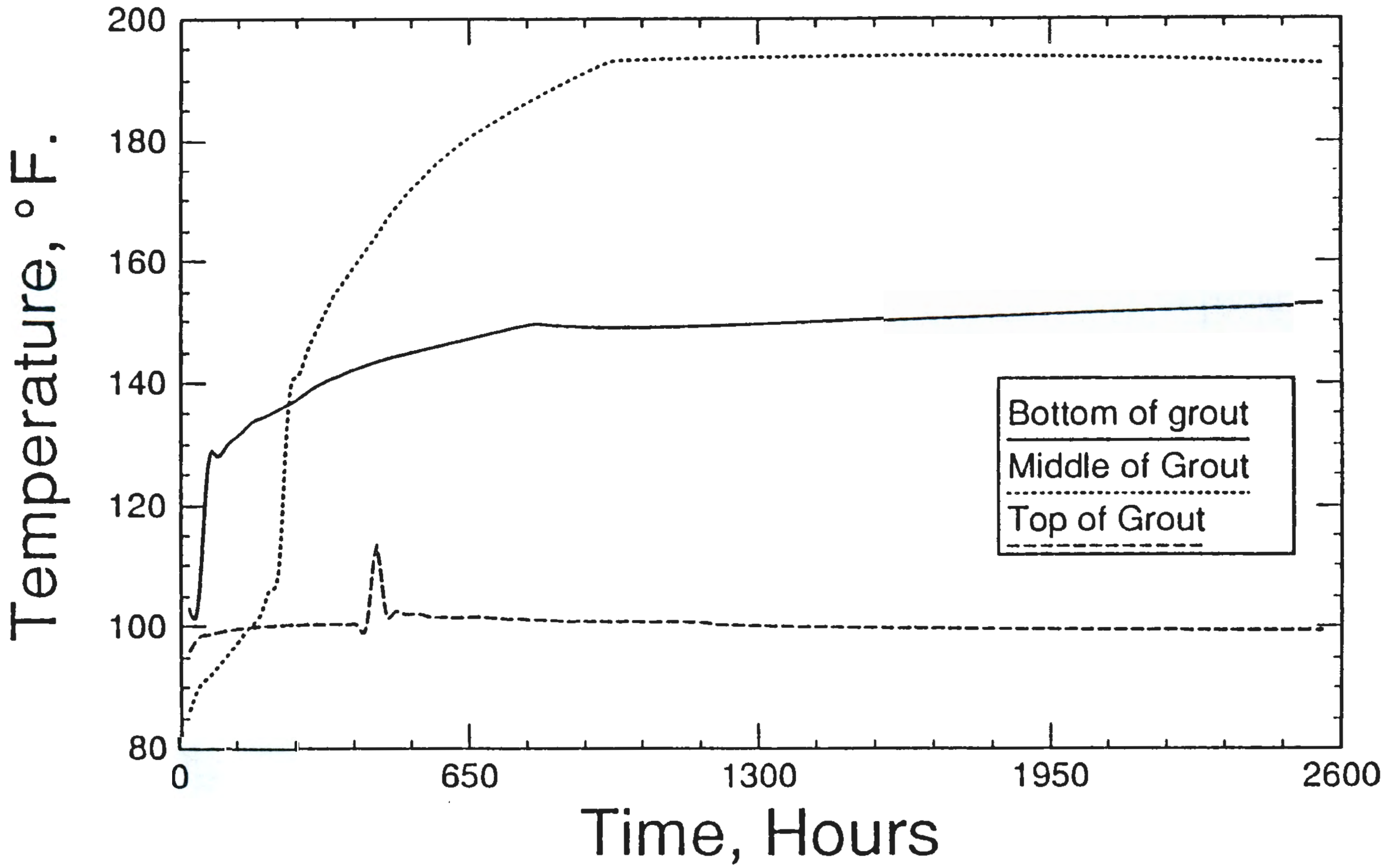

Figure 5. Grout Centerline Temperature, 2-Dimensional Model

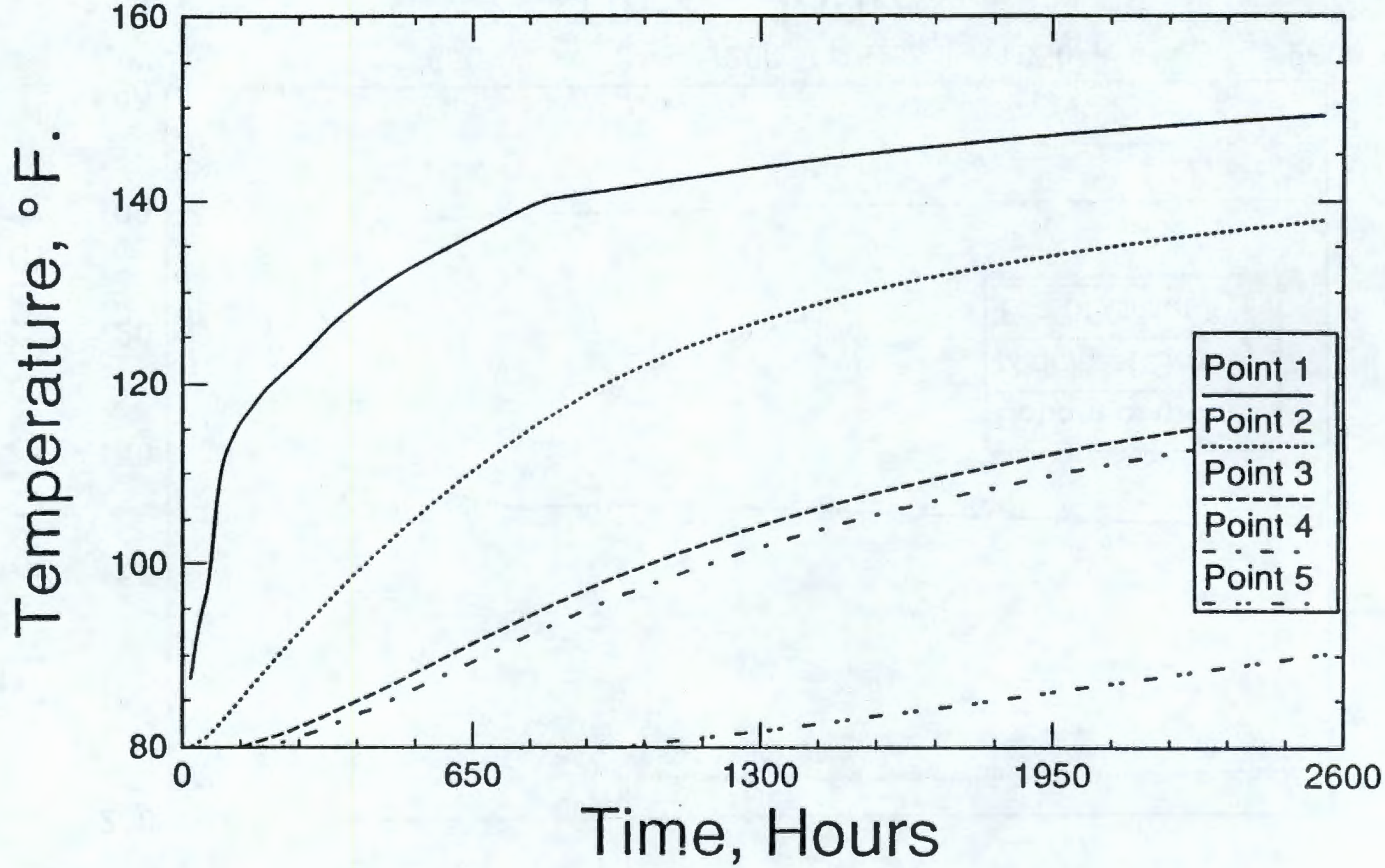

Figure 6. Vault Floor Centerline Temperature, 2-Dimensional Model

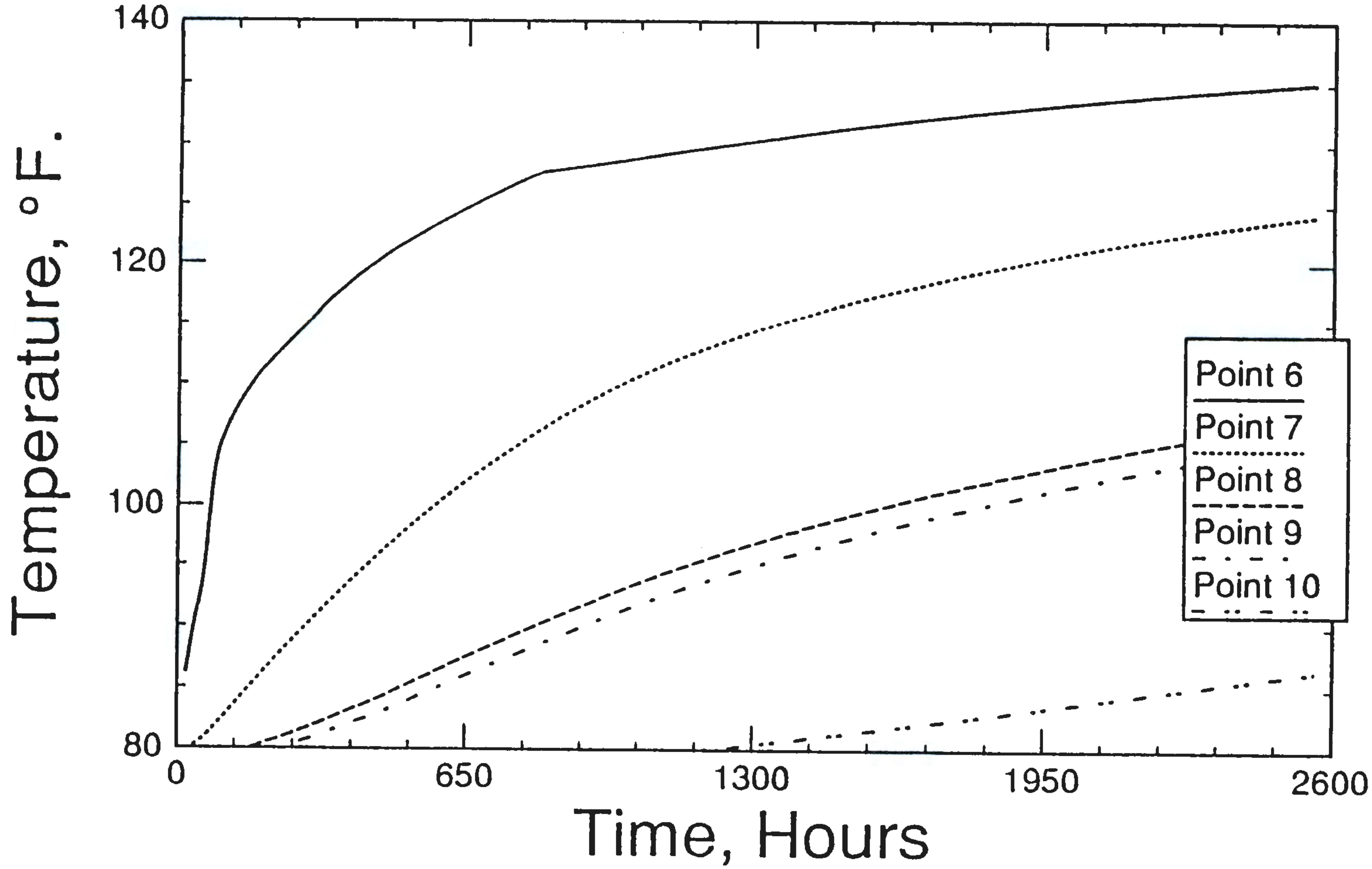

Figure 7. Vault Floor Edge Temperature, 2-Dimensional Model

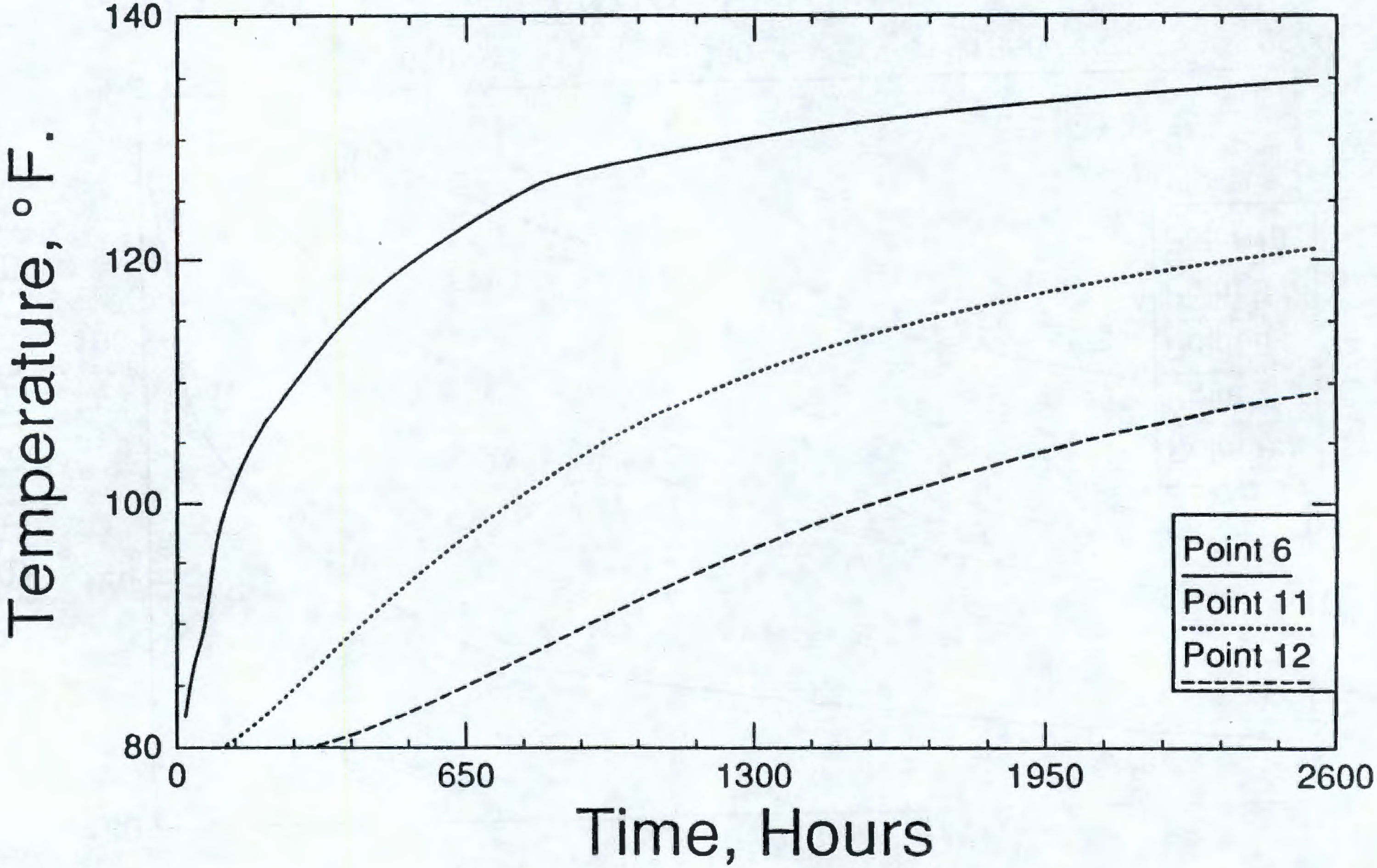

Figure 8. Vault Wall Bottom Corner Temperature, 2-Dimensional Model

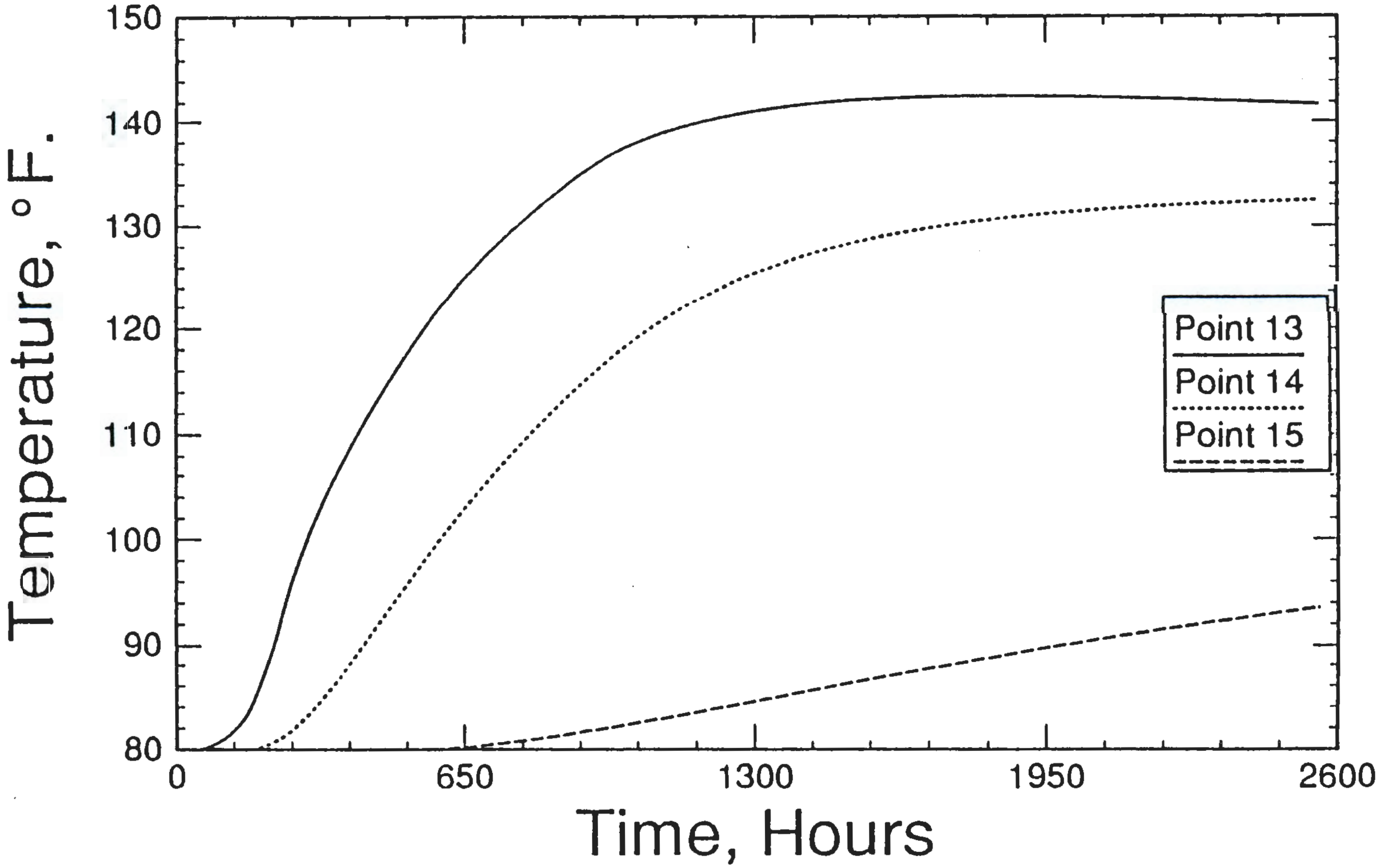

Figure 9. Wall Temperature, Grout Height = 15 Feet, 2-Dimensional Model

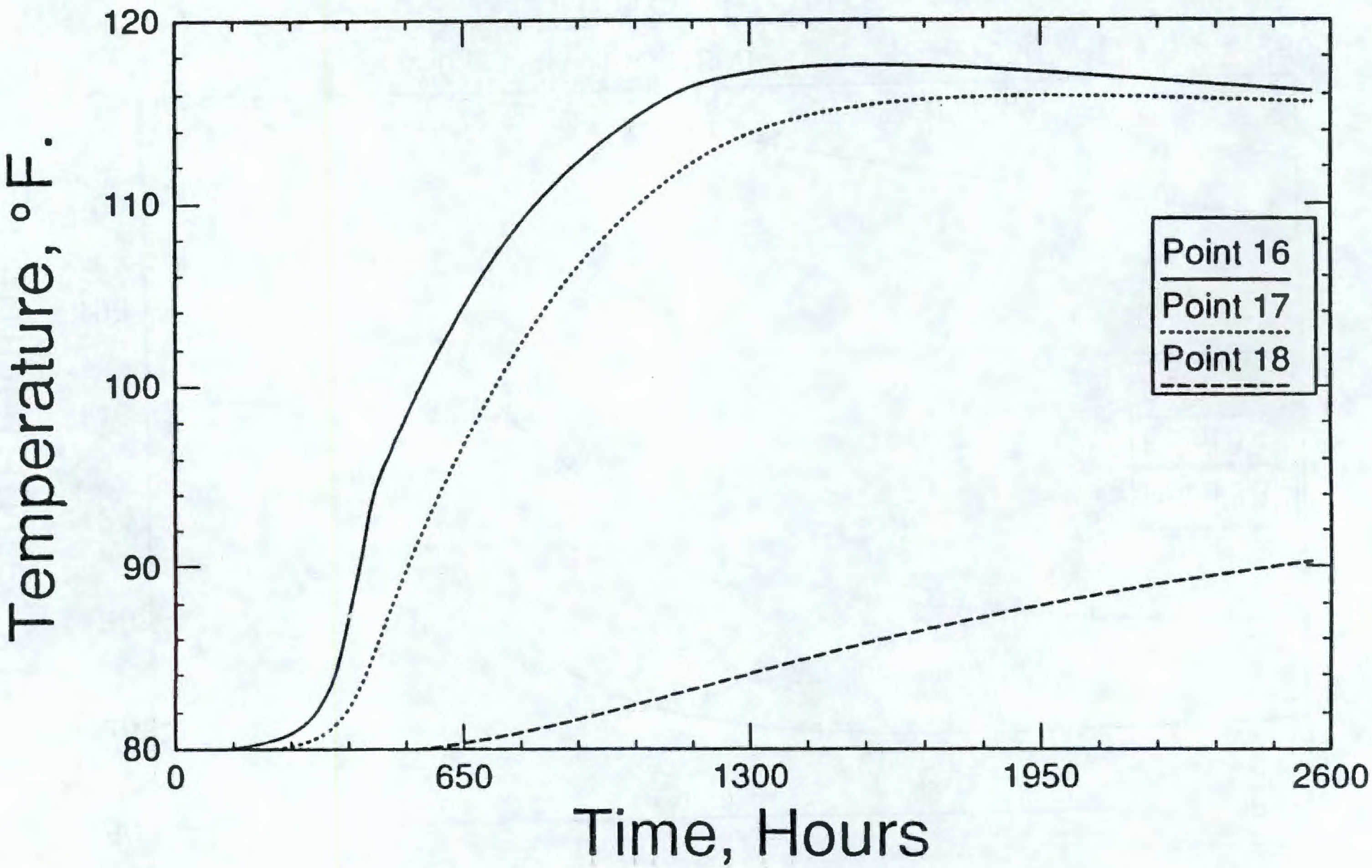

Figure 10. Wall Temperature, Grout Height = 30 Feet, 2-Dimensional Model

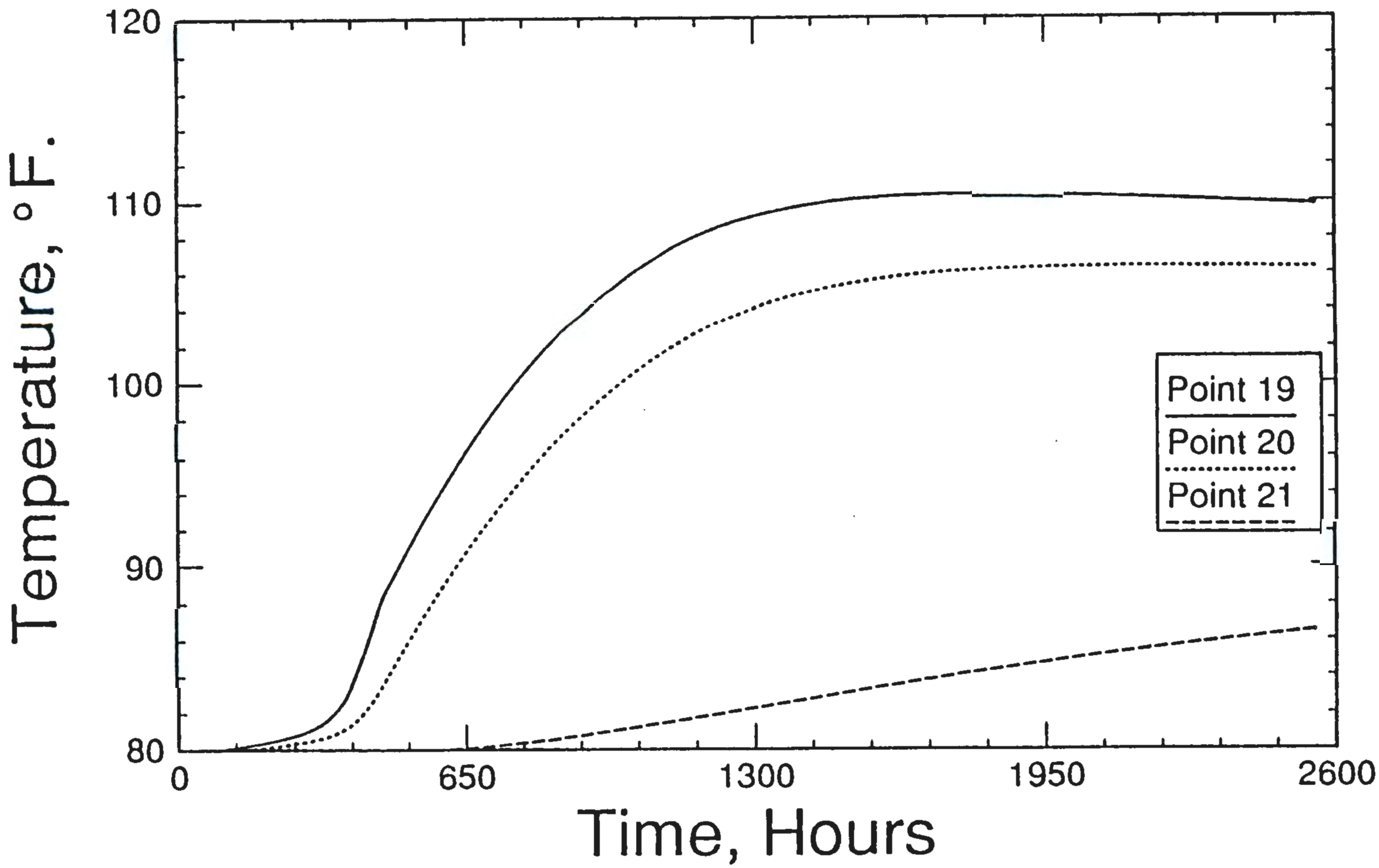

Figure 11. Wall Temperature, Top Corner, 2-Dimensional Model

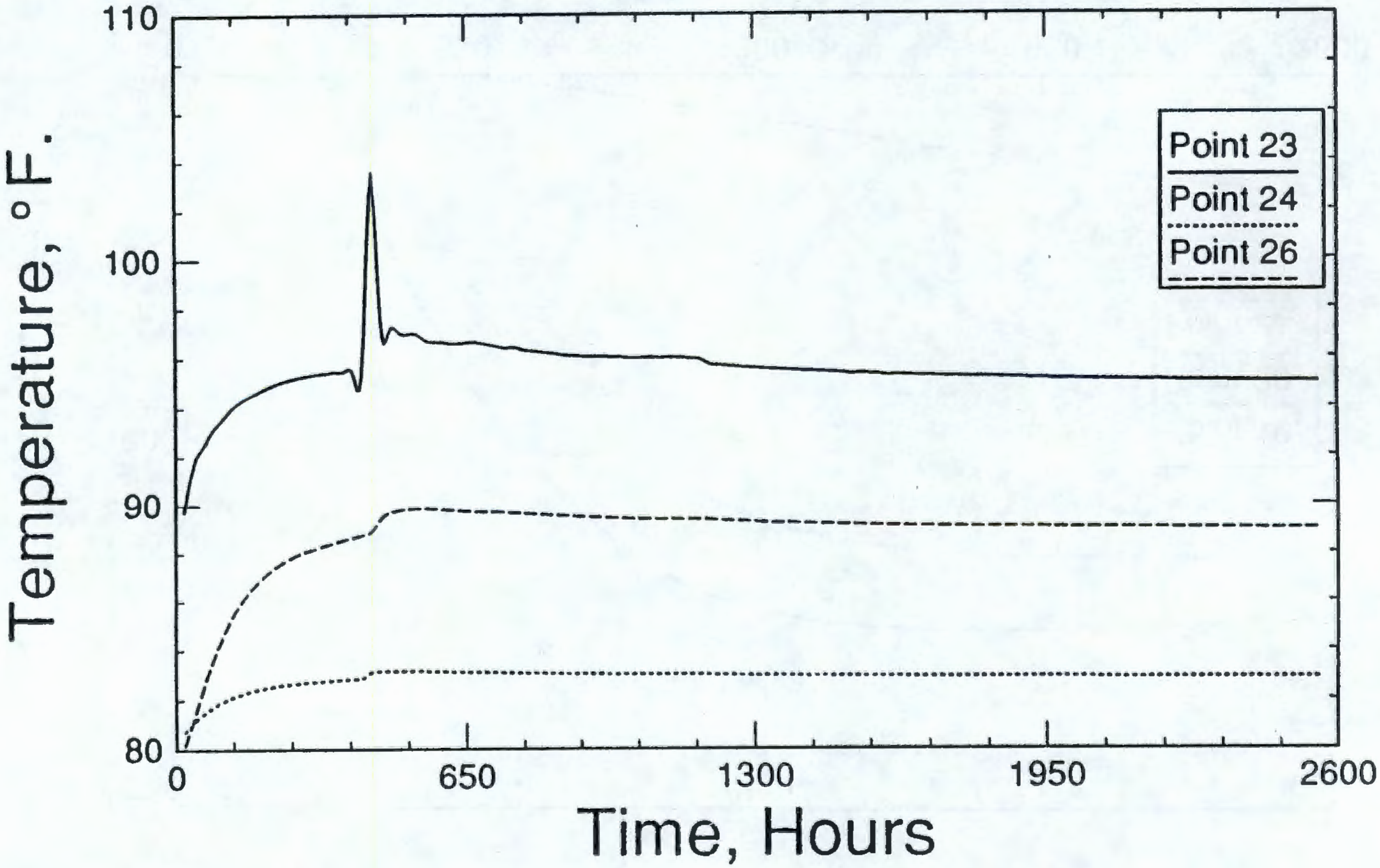

Figure 12. Coverblock Centerline Temperature, 2-Dimensional Model

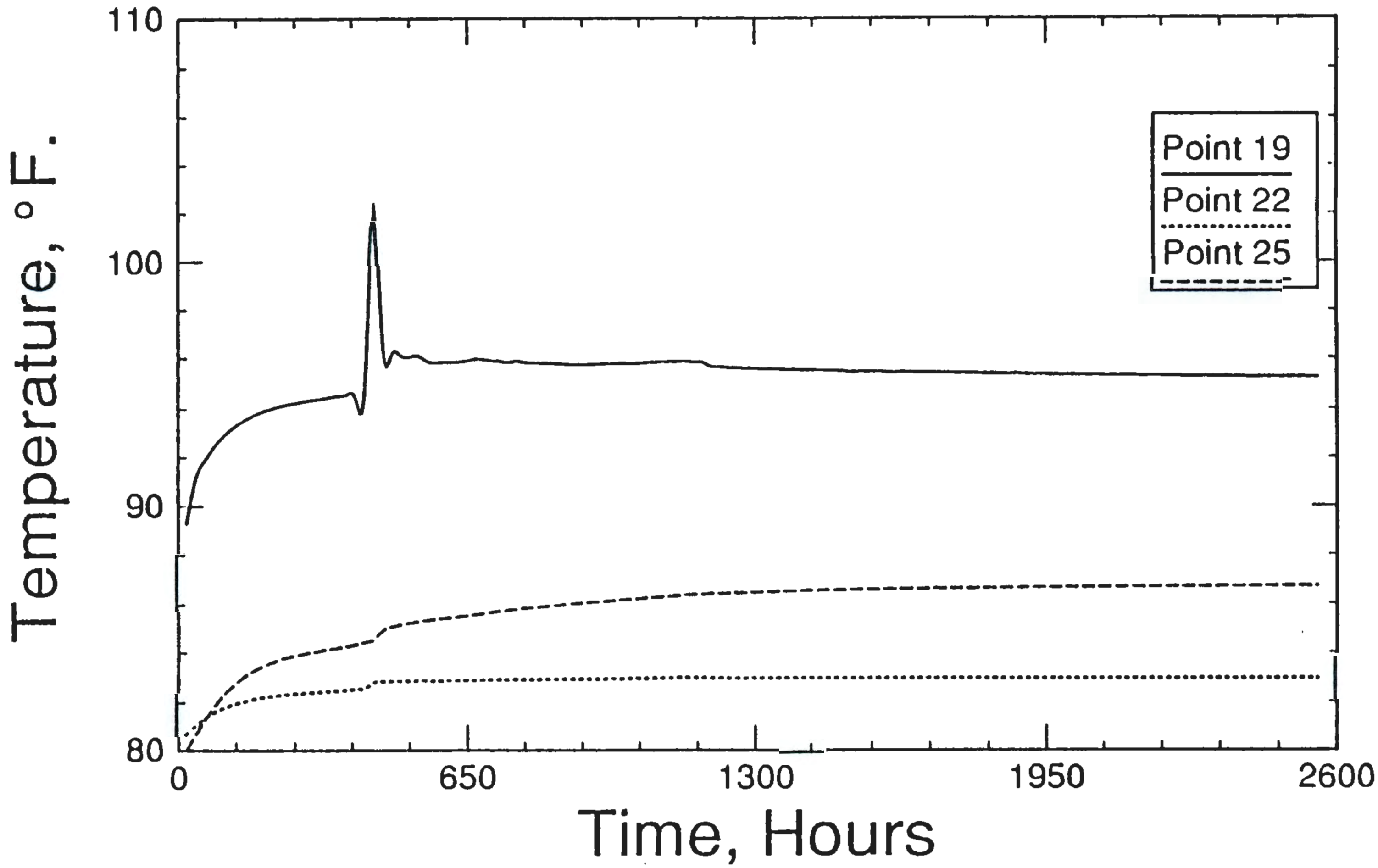

Figure 13. Coverblock Edge Temperature, 2-Dimensional Model

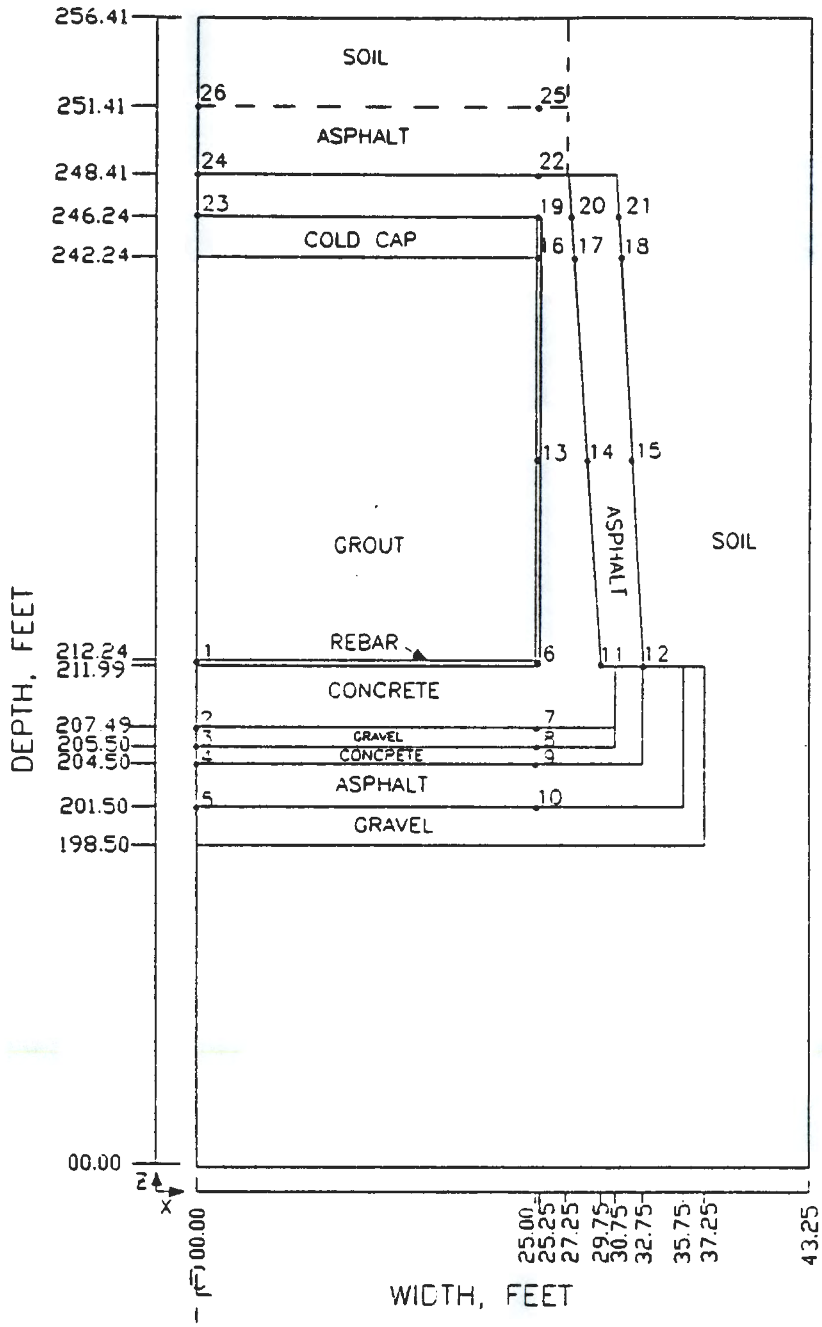

Figure 14. Asphalt Barrier Grout Vault, Temperature Gradient Point Location.

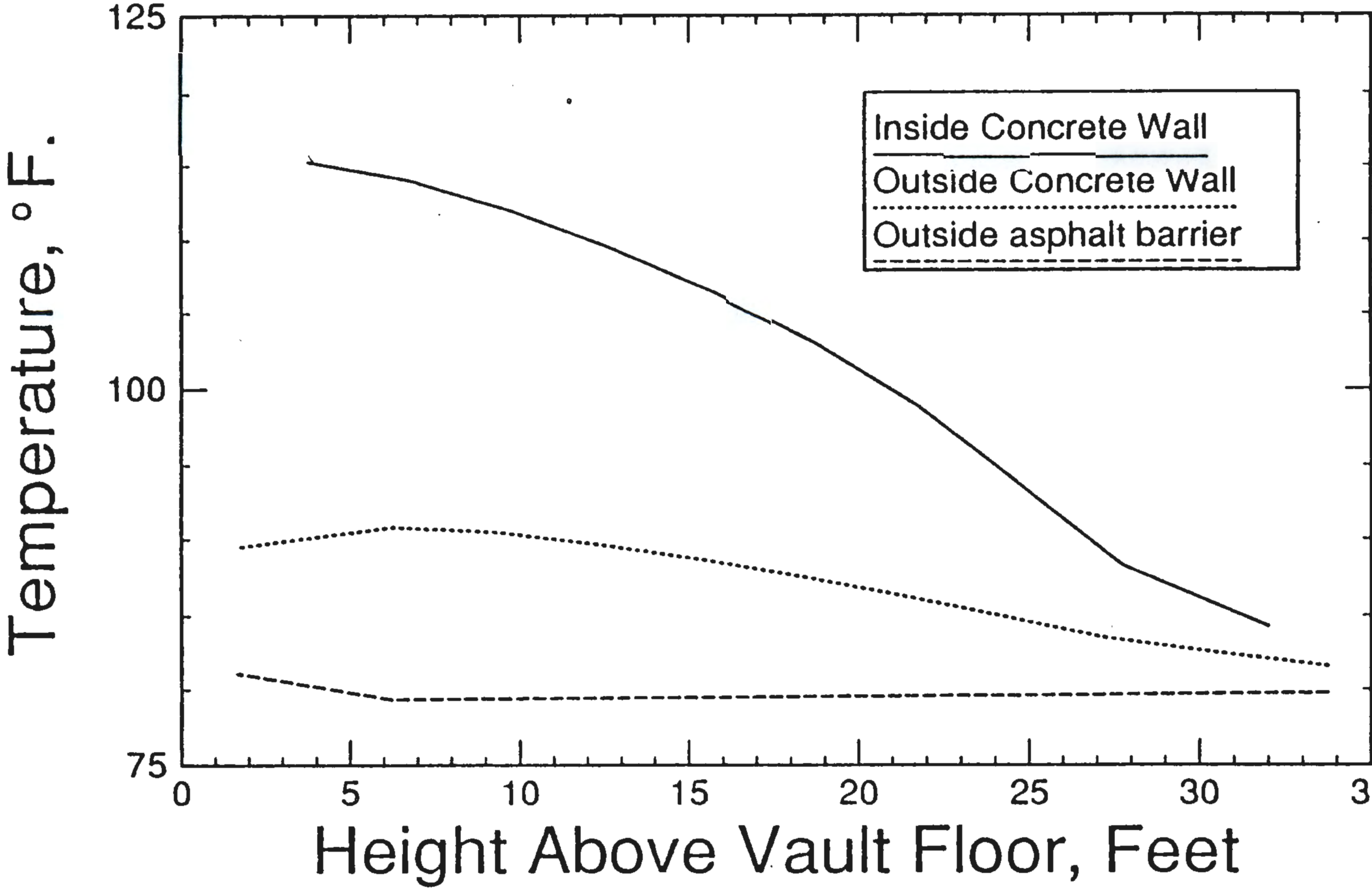

Figure 15. Vault Wall Temperatures, Time = 400 Hours, 2-Dimensional Model

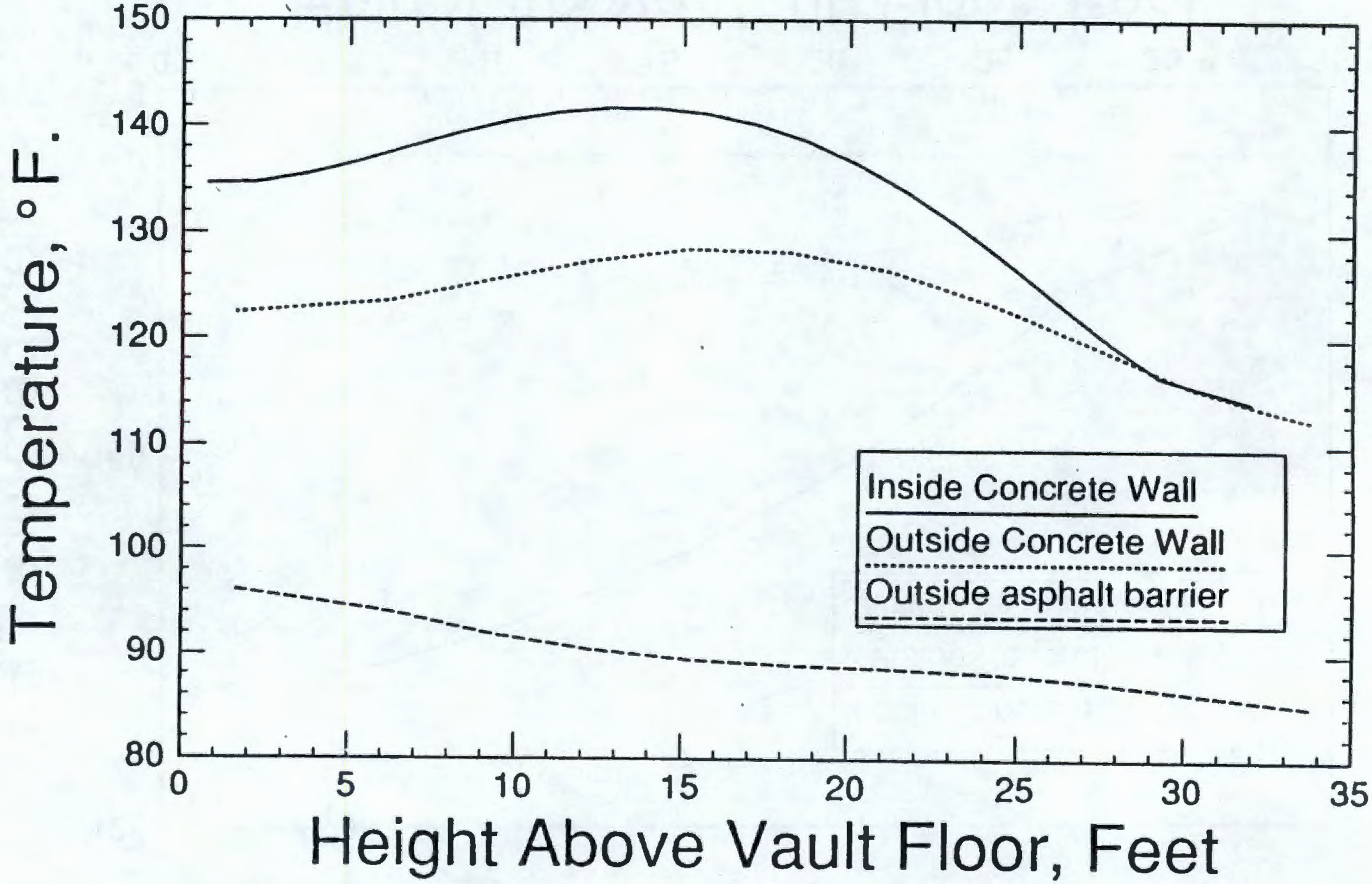

Figure 16. Vault Wall Temperatures, Time = 1880 Hours, 2-Dimensional Model

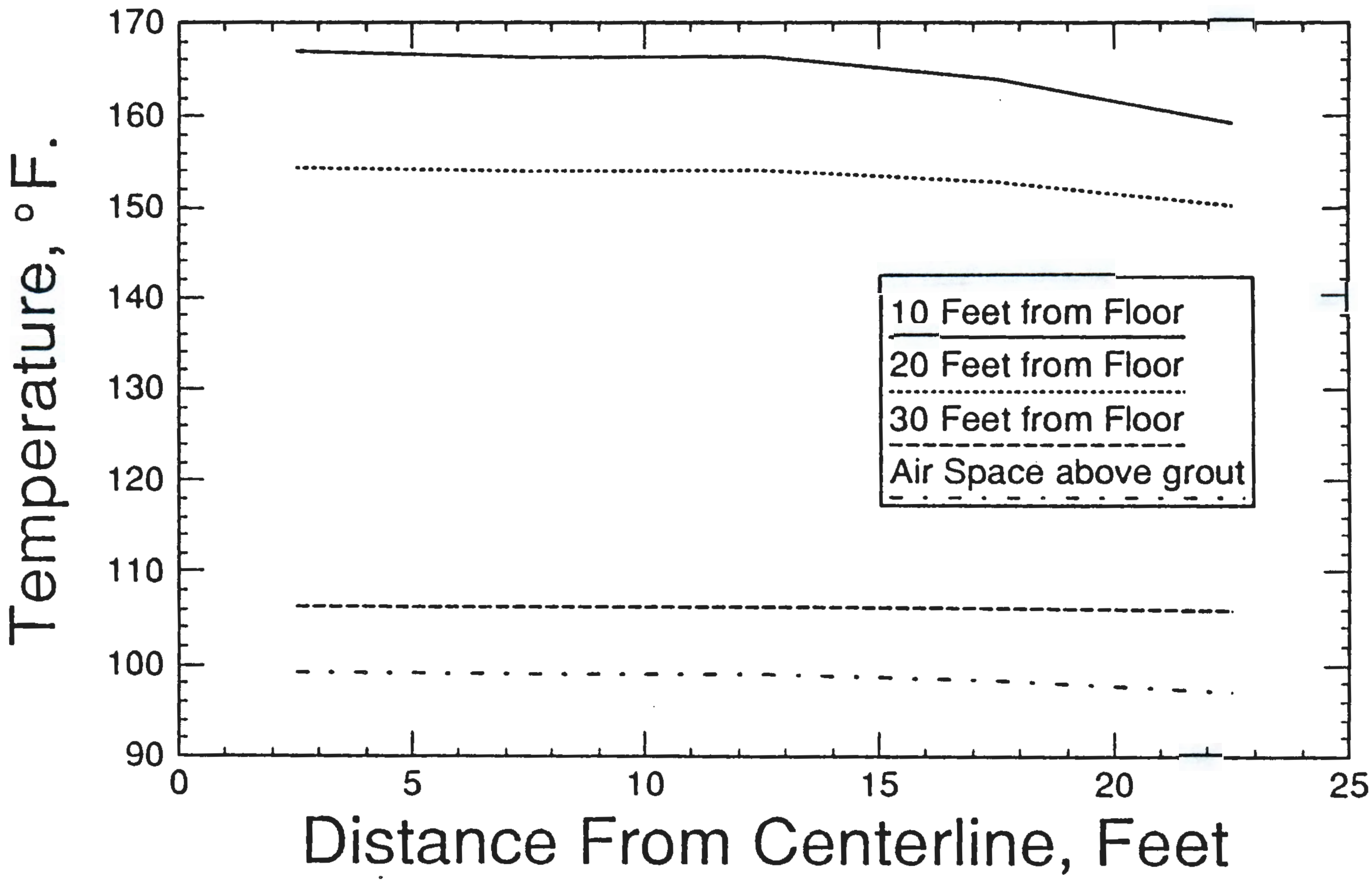

Figure 17. Vault Centerline to Wall Temperatures, Time = 400 hours, 2-Dimensional Model

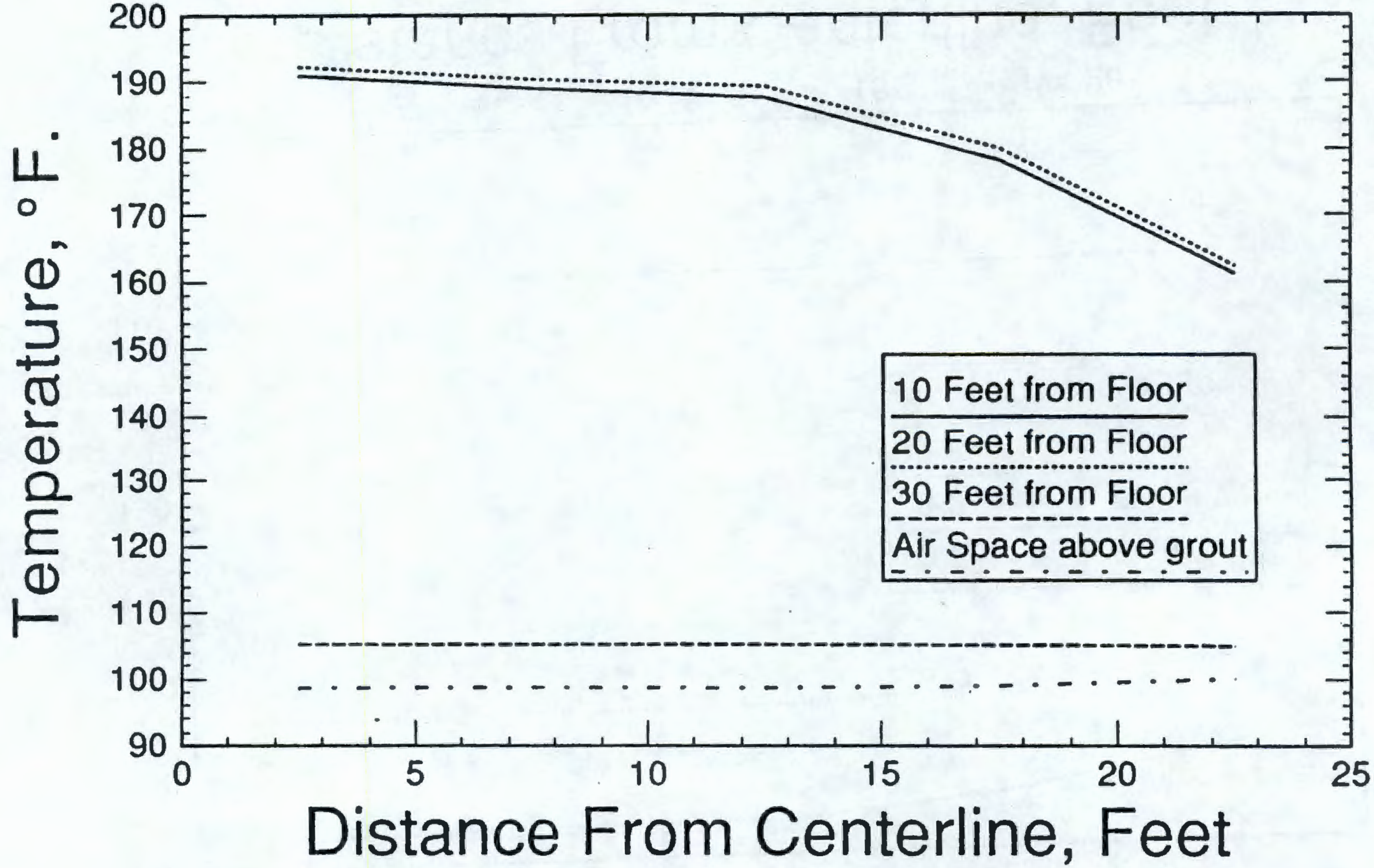

Figure 18. Vault Centerline to Wall Temperatures, Time = 1880 hours, 2-Dimensional Model

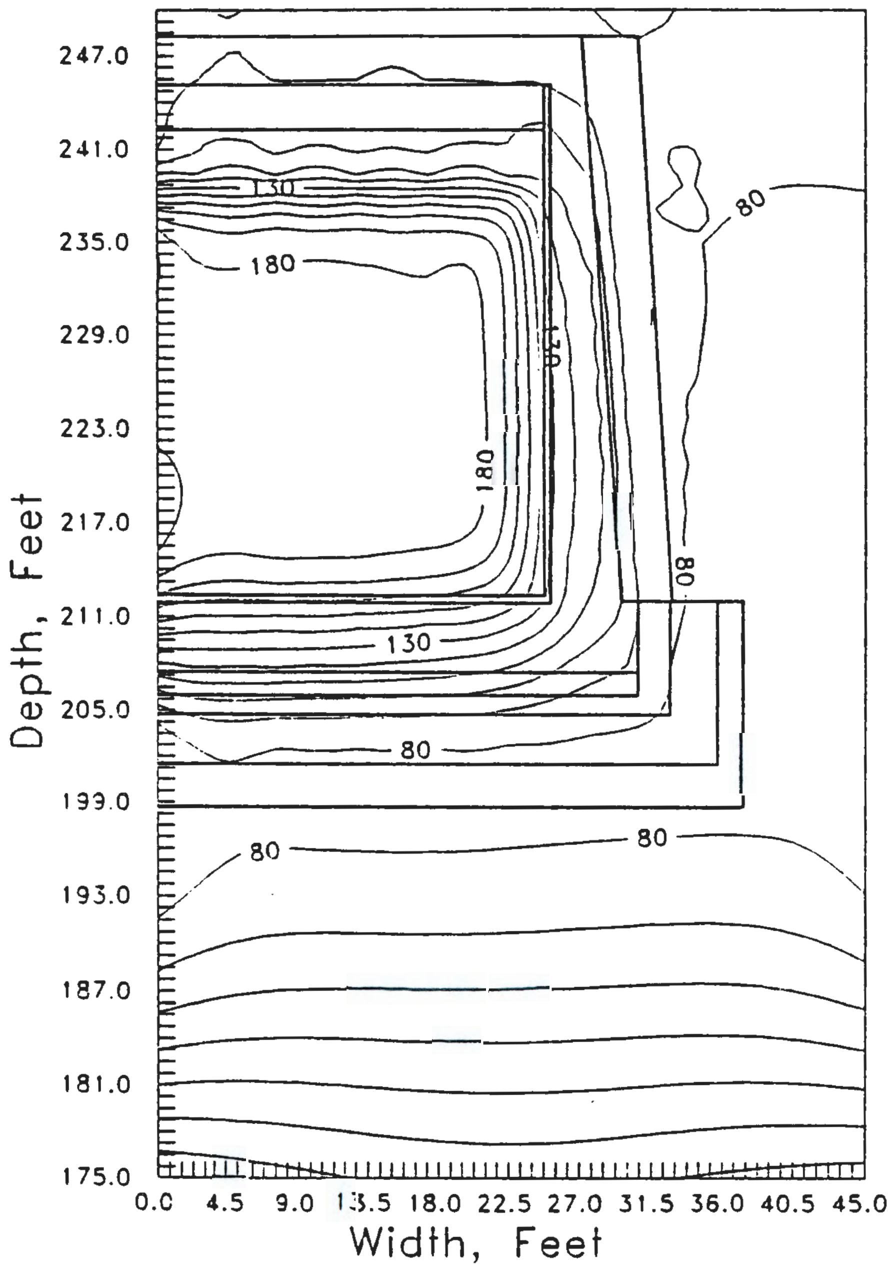

Figure 19. Temperature Contour, Full Grout Vault.

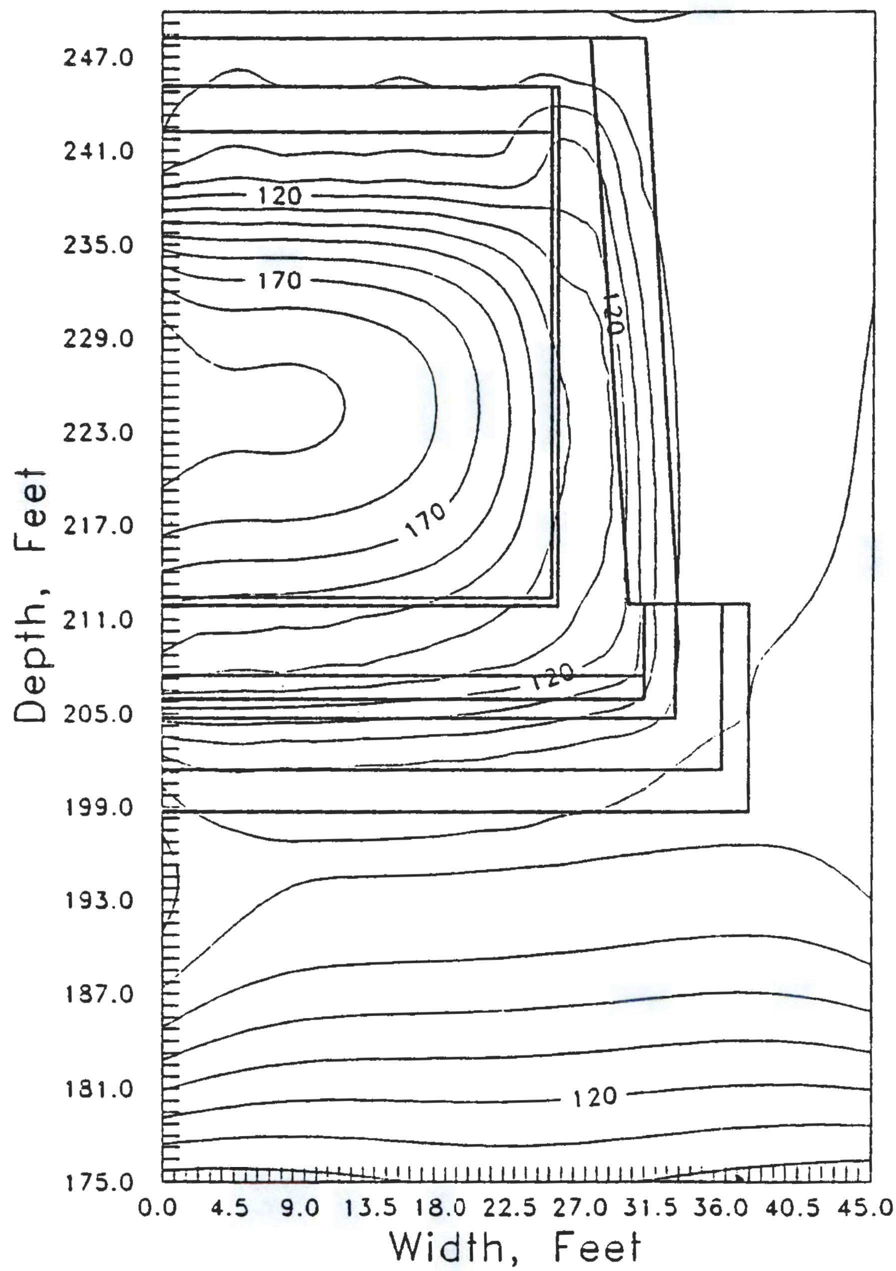

Figure 20. Temperature Contour, Three Months After Grout Vault Filled.

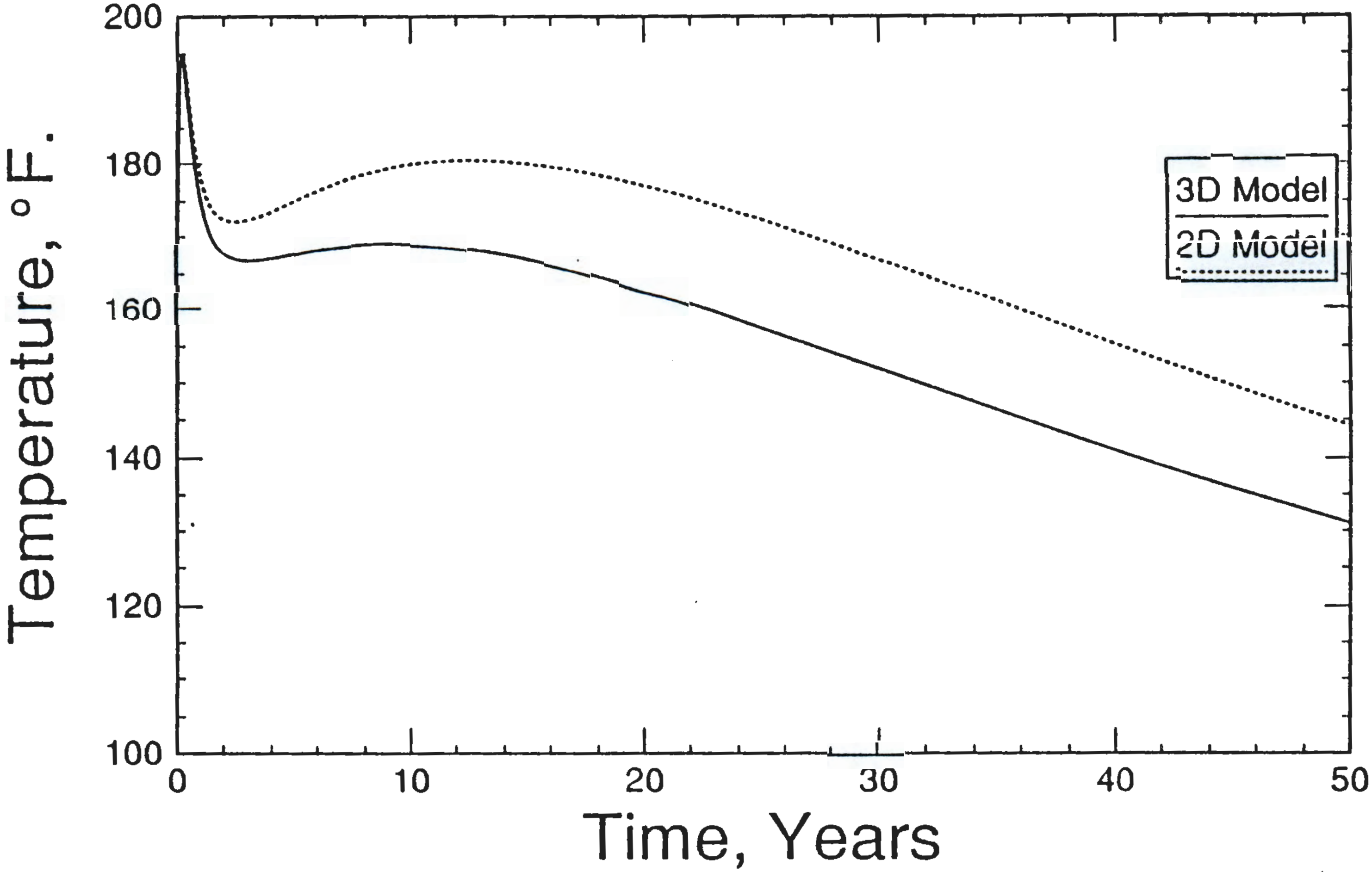

Figure 21. 2-Dimensional Versus 3-Dimensional Maximum Temperatures

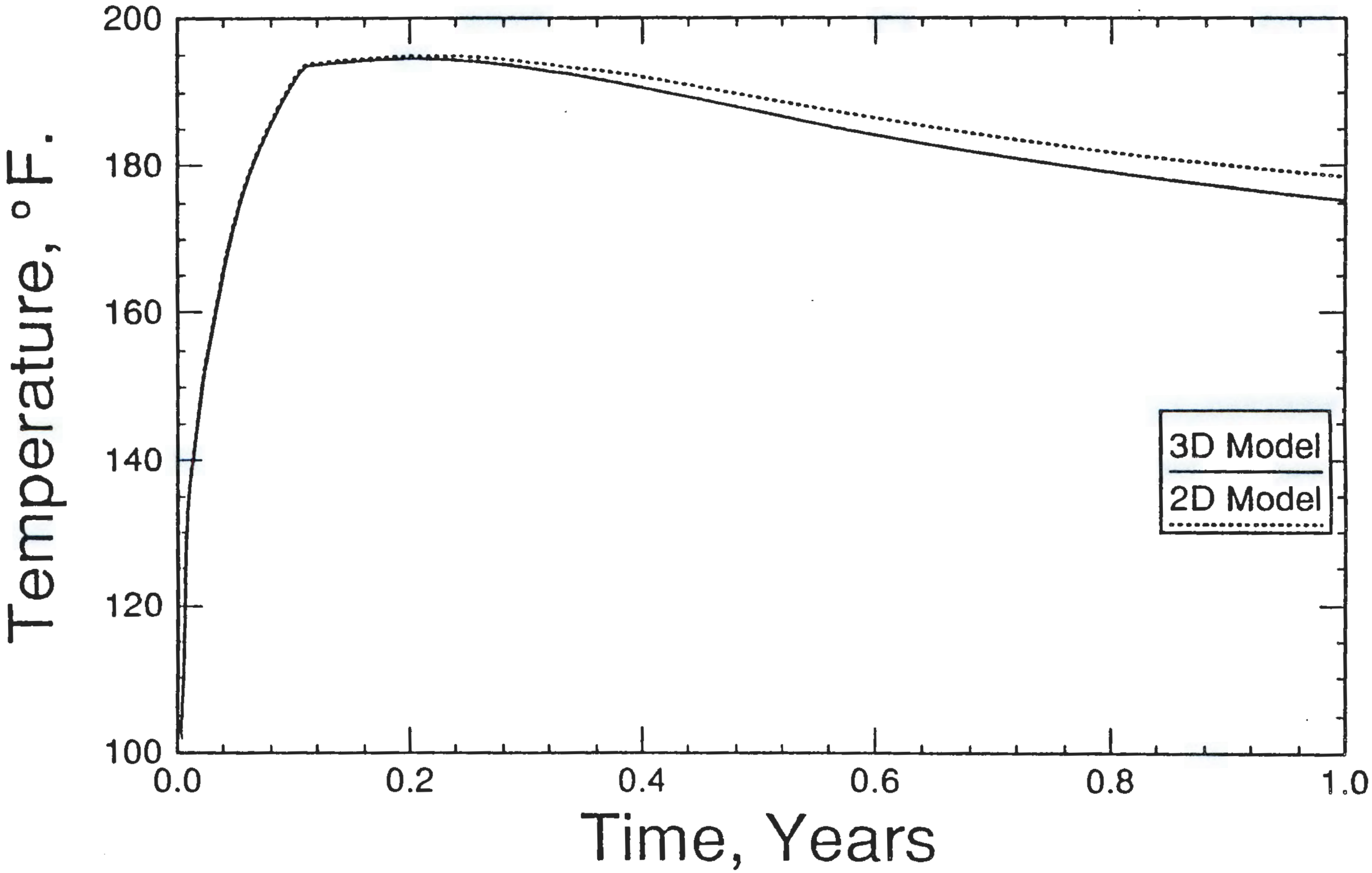

Figure 22. 2-Dimensional Versus 3-Dimensional Temperatures

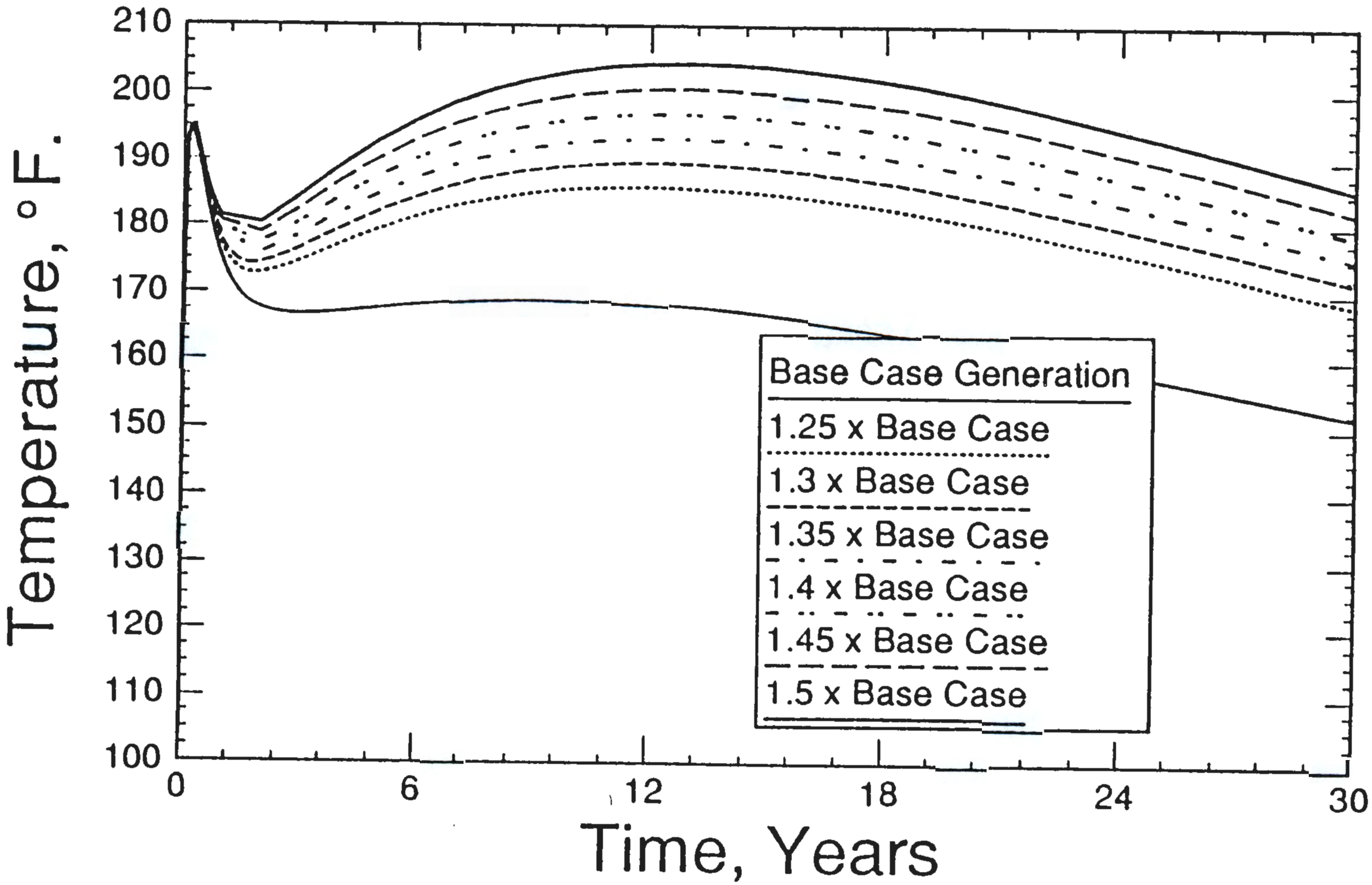

Figure 23. Radiolytic Heat Generation Curves, 3-Dimensional Model

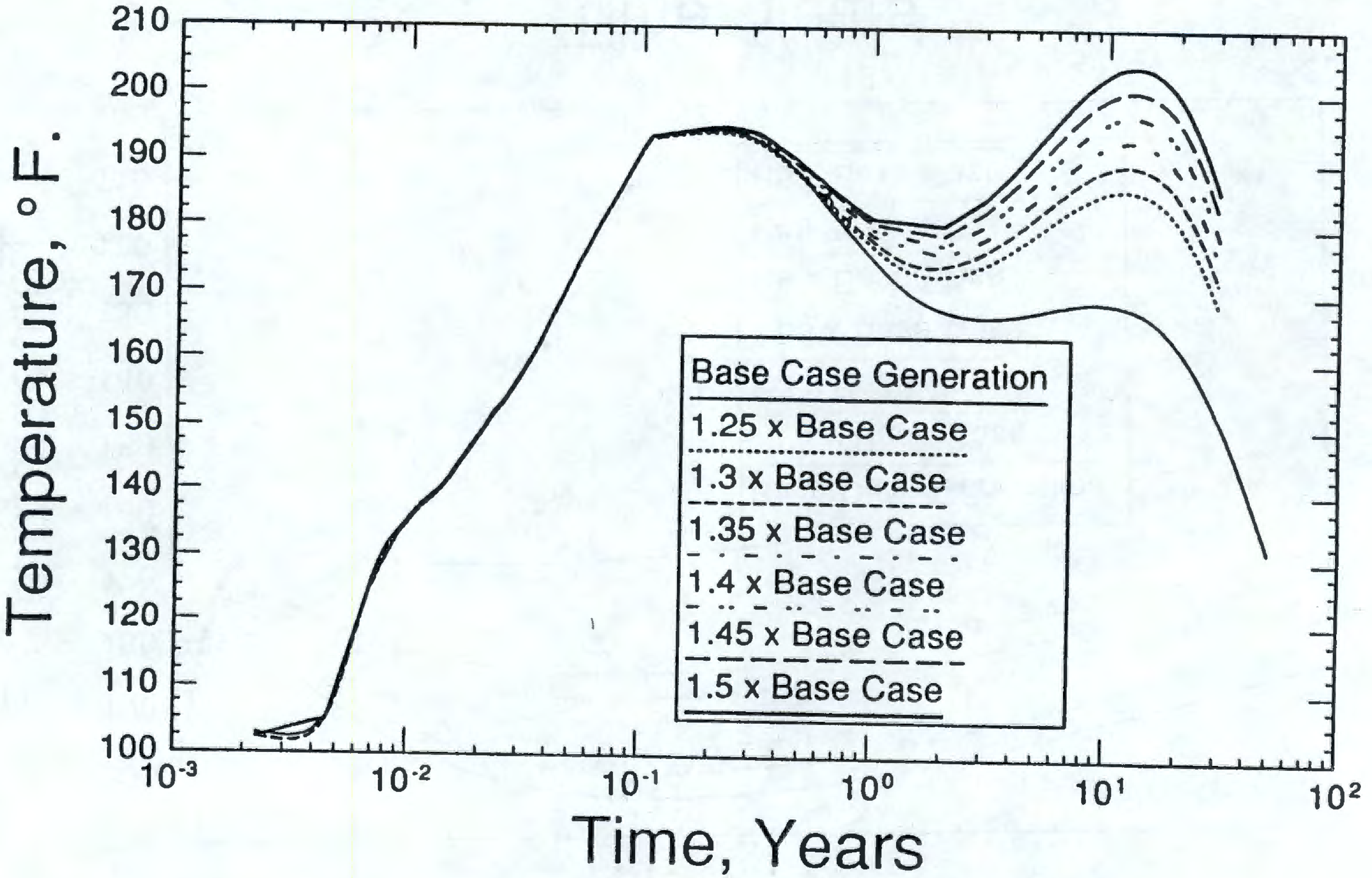

Figure 24. Radiolytic Heat Generation Curves, 3-Dimensional Model

APPENDIX A

TAPA CONTROLLING PROGRAMS

The execution of the TAPA computer code was controlled by FORTRAN programs which in turn were controlled by UNIX shell scripts. This section explains the interaction between each of these programs.

Three main FORTRAN programs were used to modify each TAPA input data file before running. The first program, tapa_init_t.f, shown in Figure A-1, loads an initial temperature distribution from a previous run into the present data file. The second program, load_12_13.f, shown in Figure A-2, loads the time corrected hydrolytic and radiolytic heat generation rates into the present data file. A second version of load_12_13.f is required for the 3-dimensional model and is shown in Figure A-3. The third program, get_if_temps.f, shown in Figure A-4, reads a TAPA output file and extracts and saves the interfacial connection data generated by the model.

This series of programs is executed in the proper order by a UNIX shell script, run_tapa, shown in Figure A-5. This script controls the execution of the TAPA runs during the vault filling stages from time period 0 through 400 hours. Execution of TAPA from 400 hours until the coverblock is covered with soil three months later is controlled by the script, run.guzek_400_2560, shown in Figure A-6.

DATA ANALYSIS PROGRAMS

Four data analysis programs were used to manipulate and extract data from the TAPA output files. The first set extracts specified interfacial temperatures from their respective data files. The second set extracts specified node or boundary temperatures from data files. The third extracts maximum temperatures and the fourth extracts node-temperature data for contour plotting. Each of these programs is discussed below.

The FORTRAN program get_if_t.f, shown in Figure A-7, extracts the temperature of a specified interfacial node pair stored in a TAPA output file. The UNIX shell script, get_interface_temperatures, shown in Figure A-8, loops this FORTRAN program so a series of time-temperature values are automatically extracted. This data is then used in various xy plots shown in the body of the report.

The FORTRAN program get_node_t.f, shown in Figure A-9, extracts the temperature of a specified internal or boundary node stored in a TAPA output file. The UNIX shell script, get_node_temperatures, shown in Figure A-10, loops this program similar to the above process to produce a file containing time-temperature data used for xy plots shown previously.

The FORTRAN program temp_tapa.f, shown in Figure A-11, reads a TAPA output file and orders the internal and boundary temperatures in descending order. The FORTRAN program tapa_max_tmp.f, shown in Figure A-12, is used in conjunction with temp_tapa.f to extract the maximum temperature-node point from the file. The UNIX shell script, get_max_tapa_temperatures, shown in Figure A-13, loops these two programs so that maximum temperature as a function of time can be created.

The FORTRAN program make_contour.f, shown in Figure A-14, reads a TAPA output file and creates a spacial temperature relationship file suitable for use with the SURFER (Reference 10) plotting package. The file xyz.dat, used by contour.f, defines the two- or three-dimensional position of each node in the model. It is not listed because the file is 2100 lines long, one line for each node point, and not germane to the present discussion.

Figure A-1
TAPA_INIT_T.F

```
      character*150 filnam,scr4_file
      character*81 line,varfor
      integer clongr

      varfor='(a81)'
      call getarg (1,filnam)
      call getarg (2,scr4_file)
      open (1,file=filnam)
      open (2,file=scr4_file)
      open (3,file='gar%bage')

      do 10 i=1,4
        read (1,varfor) line
   10 write (3,varfor) line

      read (2,varfor) line
   20 read (2,varfor,end=30) line
      if (line(1:3).eq.'015') goto 30
      write (3,varfor) line
      goto 20

   30 read (1,varfor) line
      if (line(1:12).ne.'015001.5002.') goto 30

      write (3,varfor) line

   40 read (1,varfor,end=50) line
      write (3,varfor) line
      goto 40

   50 rewind 1
      rewind 3

   60 read (3,1,end=70) line
      len=clongr(line,81)
      call dec4ar (len,varfor,3,2)
      write (1,varfor) line(1:len)
      goto 60

   70 close (3,status='delete')

    1 format (a81)
      end
```

Figure A-2
LOAD_12_13.F, TWO-DIMENSIONAL VERSION

```
      character*8 run_asci
      character*14 filnam
      character*81 line,varfor
      integer run_number,clongr
      dimension time(29),heat_gen(29)

c Loads new adiabatic and radiolytic heat values
c into the 12 and 13 card positions of the guzek_1 thru guzek_20
c and guzek_400_2560 data files assuming a 20 hour time step.
      data time / 20.,    40.,    60.,    80.,   100.,   120.,
     +   140.,   160.,   180.,   200.,   220.,   240.,   260.,
     +   280.,   300.,   320.,   340.,   360.,   380.,   400.,
     +   450.,   500.,   550.,   600.,   650.,   700.,   750.,
     +   800.,   801./
      data heat_gen/  1.1524e-6, 1.3740e-6, 1.0452e-5, 2.4672e-6,
     +       1.4995e-6, 1.3961e-6, 1.2410e-6, 1.2632e-6, 8.7904e-7,
     +       8.3472e-7, 8.4949e-7, 7.9778e-7, 8.2733e-7, 8.9381e-7,
     +       8.5688e-7, 7.3869e-7, 6.7220e-7, 5.8356e-7, 6.4266e-7,
     +       5.3924e-7, 4.7571e-7, 3.7525e-7, 3.5161e-7, 3.2207e-7,
     +       3.0138e-7, 2.8366e-7, 2.6593e-7, 1.8319e-7,       0.0/

      varfor='(a81)'

      call getarg (1,run_asci)
      call ardec4 (run_asci,8,run_number)

      if (run_number.le.20) then
          filnam='guzek_        '
          filnam(7:14)=run_asci
        else
          filnam='guzek_400_2560'
      endif

      open (1,file=filnam)
      open (2,file='new_file')

      write (*,*) '   Running the 2d version of load_12_13.'

c reads first two lines of data deck

      do 20 i=1,2
      read (1,120) line
   20 write (2,120) line

c puts the new time period in the data file
```

```
      read (1,120) line
      iend=20*run_number
      ibegin=iend-20
      line(30:43)='    -     HRS'
      call dec4ar (ibegin,line,30,4)
      call dec4ar (iend,line,35,4)
   30 write (2,120) line

c continue reading and writing the data file until
c reaching the 12 card

      read (1,120) line
      if (line(1:2).ne.'12') goto 30
      backspace (1)

c changes required between guzek_1 thru 20 and guzek_400_2560

      if (run_number.le.20) then
          max_loop=run_number
          start_time=0.
          iend=0
        else
          max_loop=20
          start_time=400.
      endif

c create the new 12 cards

      do 40 i=max_loop,1,-1
      time_interpolate=real(iend)-start_time+20*i

c linearly interpolate on time_interval

      call linear_inter (time,heat_gen,29,time_interpolate,value)
      read (1,120) line
   40 write (2,110) line(1:12),value

c create the new 13 cards

      do 45 i=1,max_loop
      time_interpolate=real(ibegin)

c calculate radiolytic heat decay based on the start of this time period

      value=1.94509e-8*exp(-2.62268e-6*time_interpolate)
      read (1,120) line
   45 write (2,110) line(1:12),value
```

```
c reads the rest of the cards in the data file

   50 read (1,120,end=60) line
      write (2,120) line
      goto 50

   60 rewind 1
      rewind 2

   70 read (2,120,end=80) line
      len=clongr(line,81)
      call dec4ar (len,varfor,3,2)
      write (1,varfor) line(1:len)
      goto 70

   80 close (2,status='delete')

  100 format (f5.0,f11.0)
  110 format (a12,1pe10.4)
  120 format (a81)
      end
```

Figure A-3
LOAD_12_13.F, THREE-DIMENSIONAL MODEL

```
      character*8 run_asci
      character*14 filnam
      character*81 line,varfor
      integer run_number,clongr
      dimension time(29),heat_gen(29)

c Loads new adiabatic and radiolytic heat values
c into the 12 and 13 card positions of the guzek_1 thru guzek_20
c and guzek_400_2560 data files assuming a 20 hour time step.
      data time / 20.,     40.,     60.,     80.,    100.,    120.,
     +   140.,    160.,    180.,    200.,    220.,    240.,    260.,
     +   280.,    300.,    320.,    340.,    360.,    380.,    400.,
     +   450.,    500.,    550.,    600.,    650.,    700.,    750.,
     +   800.,    801./
      data heat_gen/  1.1524e-6, 1.3740e-6, 1.0452e-5, 2.4672e-6,
     +     1.4995e-6, 1.3961e-6, 1.2410e-6, 1.2632e-6, 8.7904e-7,
     +     8.3472e-7, 8.4949e-7, 7.9778e-7, 8.2733e-7, 8.9381e-7,
     +     8.5688e-7, 7.3869e-7, 6.7220e-7, 5.8356e-7, 6.4266e-7,
     +     5.3924e-7, 4.7571e-7, 3.7525e-7, 3.5161e-7, 3.2207e-7,
     +     3.0138e-7, 2.8366e-7, 2.6593e-7, 1.8319e-7,       0.0/

      varfor='(a81)'

      call getarg (1,run_asci)
      call ardec4 (run_asci,8,run_number)

      if (run_number.le.20) then
          filnam='guzek_       '
          filnam(7:14)=run_asci
        else
          filnam='guzek_400_2560'
      endif

      open (1,file=filnam)
      open (2,file='new_file')

      write (*,*) '   Running the 3d version of load_12_13.'

c reads first two lines of data deck

      do 20 i=1,2
      read (1,120) line
   20 write (2,120) line

c puts the new time period in the data file
```

```
      read (1,120) line
      iend=20*run_number
      ibegin=iend-20
      line(30:43)='    -     HRS'
      call dec4ar (ibegin,line,30,4)
      call dec4ar (iend,line,35,4)
   30 write (2,120) line

c continue reading and writing the data file until
c reaching the 12 card

      read (1,120) line
      if (line(1:2).ne.'12') goto 30
      backspace (1)

c changes required between guzek_1 thru 20 and guzek_400_2560

      if (run_number.le.20) then
          max_loop=run_number
          start_time=0.
          iend=0
        else
          max_loop=20
          start_time=400.
      endif

c create the new 12 cards

      do 40 i=1,max_loop

      time_interpolate=real(iend)-start_time+20.*i

c linearly interpolate on time_interval

      call linear_inter (time,heat_gen,29,time_interpolate,value)
        do 40 j=1,3
        read (1,120) line
   40 write (2,110) line(1:12),value

c create the new 13 cards

      do 45 i=1,max_loop
      time_interpolate=real(ibegin)

c calculate radiolytic heat decay based on the start of this time period

      value=1.94509e-8*exp(-2.62268e-6*time_interpolate)
```

```
      do 45 j=1,3
      read (1,120) line
   45 write (2,110) line(1:12),value

c reads the rest of the cards in the data file

   50 read (1,120,end=60) line
      write (2,120) line
      goto 50

   60 rewind 1
      rewind 2

   70 read (2,120,end=80) line
      len=clongr(line,81)
      call dec4ar (len,varfor,3,2)
      write (1,varfor) line(1:len)
      goto 70

   80 close (2,status='delete')

  100 format (f5.0,f11.0)
  110 format (a12,1pe10.4)
  120 format (a81)
      end
```

Figure A-4
GET_IF_TEMPS.F

```
      character*150 filnam
      character*27 line
      character*58 line2
      integer clong

      call getarg (1,filnam)
      len=clong(filnam,' ')
      filnam(len+1:len+7)='_output'
      open (1,file=filnam)
      filnam(len+1:len+7)='_scr5  '
      open (2,file=filnam)

   10 read (1,100,end=40) line
      if (line.ne.'1 NODE INTERFACE CONDITIONS') goto 10

      write (2,100) line

      do 20 i=1,2
      read (1,110) line2
   20 write (2,110) line2

   30 read (1,120,err=40) i,j,k,v1,v2
      write (2,120) i,j,k,v1,v2
      goto 30

   40 continue

  100 format (a27)
  110 format (a58)
  120 format (i12,2i10,f12.2,e14.4)
      end
```

Figure A-5
RUN_TAPA

```
i=$1

# shell script for running the first 20 tapa a cases
# $1 is the starting number and $2 is the finishing number

while test $i -le $2
   do echo Starting guzek_$i
      last=`expr $i - 1`
      tapa_init_t guzek_$i guzek_${last}_scr4
      load_12_13 $i
      tapa guzek_$i
      rm guzek_${i}_scr1
      rm guzek_${i}_scr2
      rm guzek_${i}_scr3
      get_if_temps guzek_$i
      rm guzek_${i}_output
      i=`expr $i + 1`
done
```

Figure A-6
RUN.GUZEK_400_2560

```
i=21

##################################################################
# This shell script controls the 400 to 2560 time period
# of the grout pour. It uses guzek_400_2560 as its data file
# and changes the adiabatic and radiolytic heat generation
# rate every 20 hours.  Only the "scr4" files are saved on
# each run.  They are stored in "guzek_21_scr4" thru
# "guzek_128_scr4".
##################################################################

while test $i -le 128
  do echo Starting guzek_${i}.
    last=`expr $i - 1`
    tapa_init_t guzek_400_2560 guzek_${last}_scr4
    load_12_13 $i
    tapa guzek_400_2560
    cp guzek_400_2560_scr4 guzek_${i}_scr4
    get_if_temps guzek_400_2560
    mv guzek_400_2560_scr5 guzek_${i}_scr5
    i=`expr $i + 1`
done

rm guzek_400_2560_scr*
rm guzek_400_2560_output
```

Figure A-7
GET_IF_T.F

```
      integer strlen,sklong
      character*200 filnam,node_name

c program reads a tapa "scr5" file and picks the desired
c temperature of the specified node i - j pair

c the first argument is the file name
c the second argument is the node i number
c the third argument is the node j number

      call get_datafile (filnam,len_filnam,1)

      iend=sklong(filnam,2,'_')-1
      call ardec4 (filnam(7:iend),iend-7,itime)
      itime=itime*20.

      call get_arg (2,node_name,strlen)
      call ardec4 (node_name,strlen,node_i)

      call get_arg (3,node_name,strlen)
      call ardec4 (node_name,strlen,node_j)

   10 continue
      read (1,100,end=30,err=10) n_i,n_j,temp
      if (n_i.ne.node_i.and.n_j.ne.node_j) goto 10

      write (*,110) itime,temp

   30 continue

  100 format (12x,2(i10),,f12.0)
  110 format (i5,f10.2)

      end
```

Figure A-8
GET_INTERFACE_TEMPERATURES

```
i=$1
rm interface_temperatures
# shell script for getting interfacial temperatures
# $1 is the starting data file and $2 is the finishing
# data file

while test $i -le $2
   do get_if_t guzek_${i}_scr5 $3 $4>>interface_temperatures
      i=`expr $i + 1`
done
```

Figure A-9
GET_NODE_T.F

```
      dimension temp(6000),this_line(6),node_no(6000)
      integer start_node,first_card,strlen,sklong
      character*200 filnam,node_name

c program reads a tapa input file or a "scr4" file and
c picks the desired temperature of the specified internal node
c or boundary node

c the first argument is the file name
c the second argument is the node number
      call get_datafile (filnam,len_filnam,1)

      iend=sklong(filnam,2,'_')-1
      call ardec4 (filnam(7:iend),iend-7,itime)
      itime=itime*20.

      call dec4ar (len_filnam,varfor,3,3)
      call get_arg (2,node_name,strlen)
      call ardec4 (node_name,strlen,node_number)

      ilines=0
   10 continue
      read (1,100,end=30,err=10) first_card,start_node,this_line
      if (first_card.ne.1) goto 10

      ilines=ilines+1

      do 20 i=1,6
      node_no((ilines-1)*6+i)=start_node-1+i
      if (this_line(i).gt.0.) then
          temp((ilines-1)*6+i)=this_line(i)-459.69
        else
          temp((ilines-1)*6+i)=this_line(i)
      endif
   20 continue
      goto 10

   30 max=ilines*6

      if (node_number.eq.node_no(node_number)) then
          write (*,110) itime,temp(node_number)
        else
          do 40 i=1,max
          if (node_no(i).eq.node_number)
     +    write (*,110) itime,temp(i)
```

```
 40     continue
    endif

100 format (i2,i4,6x,6(f10.0))
110 format (i5,f10.2)

          end
```

Figure A-10
GET_NODE_TEMPERATURES

```
i=$1
rm node_temperatures
# shell script for getting node temperatures
# $1 is the starting data file and $2 is the finishing
# data file, $3 is the node number

while test $i -le $2
   do $COM_EXE/get_node_t guzek_${i}_scr4 $3 >>node_temperatures
      i=`expr $i + 1`
done
```

Figure A-11
TEMP_TAPA.F

```
      dimension temp(6000),this_line(6)
      real node_no(6000)
      integer start_temp,first_card
      character*200 filnam

c program reads a tapa input file or a "scr4" file and
c orders the node temperatures in descending temperature
c order

      call get_datafile (filnam,len_filnam,1)

      ilines=0
   10 continue
      read (1,100,end=30,err=10) first_card,start_temp,this_line
      if (first_card.ne.1) goto 10

      ilines=ilines+1
      do 20 i=1,6
      node_no((ilines-1)*6+i)=start_temp-1+i
      if (this_line(i).gt.0.) then
          temp((ilines-1)*6+i)=this_line(i)-459.69
        else
          temp((ilines-1)*6+i)=this_line(i)
      endif
   20 continue
      goto 10

   30 max=ilines*6

      open (2,file='jun#k')
      call ssort (temp,node_no,max,-2)
      write (2,110 ) (node_no(i),temp(i),i=1,max)

  100 format (i2,i4,6x,6(f10.0))
  110 format (f5.0,5x,f10.2)

      end
```

Figure A-12
TAPA_MAX_TMP.F

```
      character*50 line

      open (1,file='jun#k')
      read (1,2) line
      open (2,file='jun#k_2')
      write (2,2) line

    2 format (a50)

      end
```

Figure A-13
GET_MAX_TAPA_TEMPERATURES

```
rm -f max_tapa_temps

# Script reads the "scr4" data files starting at $1 and ending
# at $2 and writes the maximum temperatures to the file
# "max_tapa_temps"

start=$1
end=$2

while test $start -le $end
   do temp_tapa guzek_${start}_scr4
      tapa_max_tmp
      echo guzek_${start}>>max_tapa_temps
      cat jun#k_2>>max_tapa_temps
      start=`expr $start + 1`
done

rm jun#k
rm jun#k_2
```

Figure A-14
MAKE_CONTOUR.F

```
      dimension temp(2100)
      real node(2100),x(2100),y(2100),z(2100),temp(2110)
      character*80 line
      character*200 filnam

c opens the xyz - node number file

      open (1,file='xyz.map')

      do 10 i=1,2100
   10 read (1,100,end=20) node(i),x(i),y(i),z(i)

c opens the tapa "scr4" file to use

   20 close (1)
      max_nodes=i-1

      call get_datafile (filnam,len,1)
      open (1,file=filnam)

c the second argument is the requested z slice

      call getarg (2,filnam)
      call ascifp (filnam,20,y_value)

      read (1,11) line

      do 30 i=1,5000
      j=(i-1)*6+1
      read (1,110,end=40) value,temp(j),
     +                          temp(j+1),
     +                          temp(j+2),
     +                          temp(j+3),
     +                          temp(j+4),
     +                          temp(j+5)
   30 if (value.ge.3000) goto 40

   40 close (1)
      open (1,file='contour.fil')

      do 50 i=1,max_nodes
      j=int(node(i))
      temp(j)=temp(j)-459.7
   50 if (y(i).eq.y_value) write (1,101) x(i)/12.,z(i)/12.,temp(j)
```

```
 11 format (a80)
100 format (4f10.2)
101 format (3f10.2)
110 format (2x,f4.0,6x,6(f10.0))

    end
```

APPENDIX B

SELECTED REFERENCES

REFERENCE 7

MEETING MINUTES

MEETING MINUTES

Subject: HEAT OF HYDRATION OF THE RE-FORMULATED GROUT

TO:	* G. K. Allen	R3-63		B. R. Dickey	R1-48
	* S. C. Chang	R1-48	*	J. C. Guzek	H0-34
	* R. D. Claghorn	R1-48	*	R. O. Lokken	P8-37
	* B. A. Crea	H0-33		J. A. Voogd	R1-48
	* Attendees			G. F. Williamson	R1-48

FROM: S. C. Chang/R. D. Claghorn CHAIRMAN: S. C. Chang

Dept-Operation-Component	Area	Shift	Meeting Date	# Attending
			1/22/90	6

The purpose of the meeting was to discuss the application of the most recent calorimetry data from the Pacific Northwest Laboratory (PNL). This data shows an adiabatic temperature rise of at least 43° C. Assuming that the starting temperature for the grout is 45° C, the centerline grout temperature in the vault will be very near the 90° C limit.

Ryan Lokken explained how the data was obtained and how the test equipment was calibrated. Blaine Crea then presented his calculation of heat loss from the equipment. Ryan showed some empirical data for heat loss that appears to be very consistent with Blaine's calculation.

The attendees came to the following conclusions and recommendations:

EVALUATION OF EXISTING THE TEST DATA:

1. The error associated with the data is +/- 5° C at the end of the test (see attached Figure, provided by Blaine Crea).

2. The test was stopped before the grout temperature reached its peak.

3. Extrapolation of the data shows that the total adiabatic temperature increase is near, if not beyond, the 45° C limit.

4. Other uncertainties, such as the effect of dry material variability and the effect of waste composition, may affect the adiabatic temperature rise.

RECOMMENDATIONS:

1. Repeat the test with improved equipment, test procedure and error analysis. This recommendation confirms the need for the new equipment that Ryan has been assembling for future tests. Terminate future tests only after the temperature rise reaches its peak.

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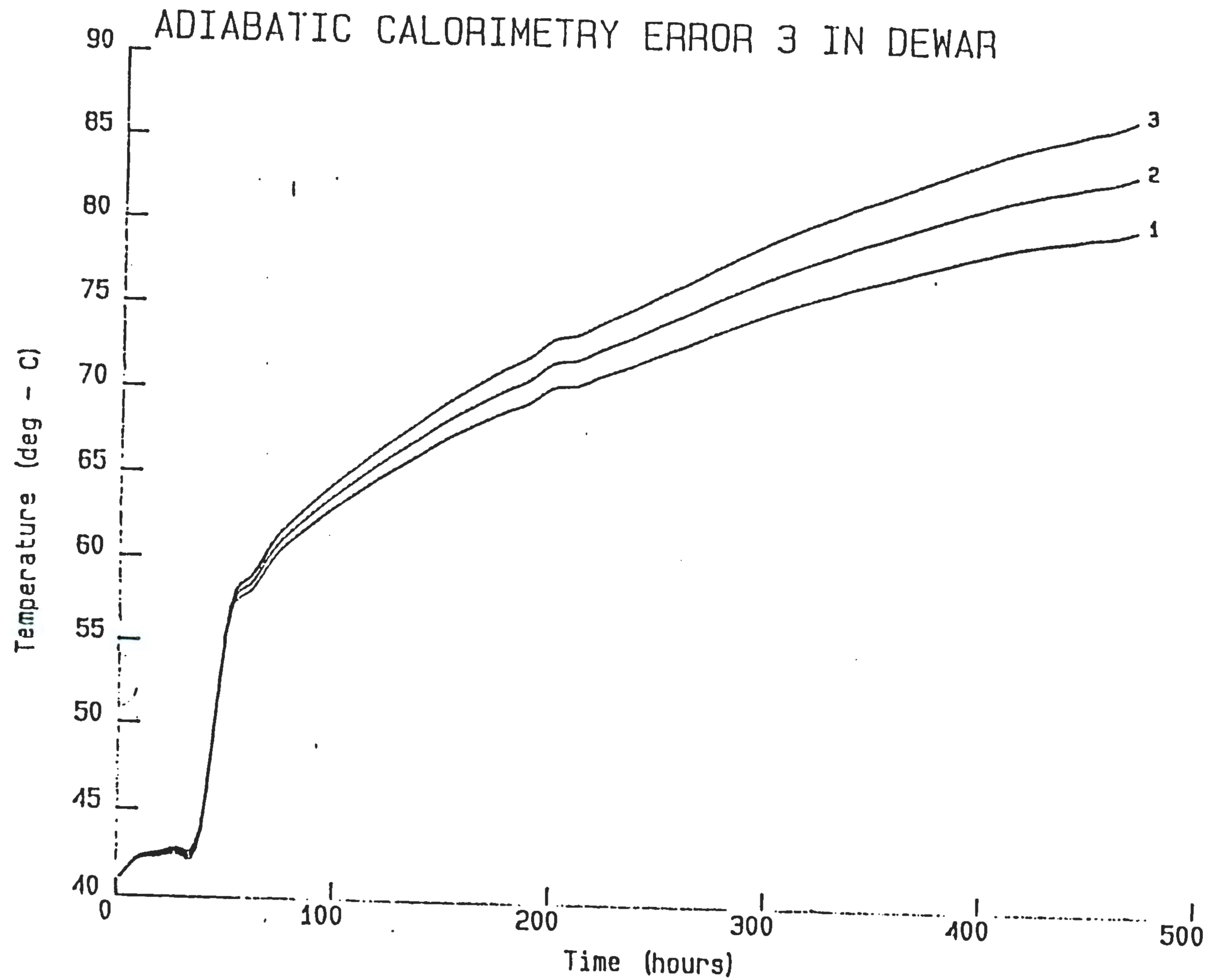
2. Perform isothermal calorimetry at Oak Ridge National Laboratory (ORNL). This recommendation confirms the need for tests that are currently in ORNL's work scope.

3. The reformulated grout (alone) may not meet the needs of the grout disposal program. Tight controls on waste feed temperature and/or dry material composition may be required. The PNL is currently conducting tests to verify grout quality up to 95° C. Due to the slow heat release of the re-formulated grout, the slow pouring process is no longer a practical option.

4. Quantify the uncertainty of the adiabatic temperature rise as a function of dry material variability, initial temperature and waste composition. This confirms the need for the tests that are currently planned for this year.

5. Validate laboratory data and thermal analyses with a pilot pour. This confirms the need for the pilot pour that is tentatively scheduled for the fall of 1990.


ADIABATIC CALORIMETRY ERROR 3 IN DEWAR
Temperature (deg - C)
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85
80
75
70
65
60
55
50
45
40
0
100
200
300
400
500
Time (hours)
3
2
1